

# Simulating battery materials on a chemistry platform for quantum computers

**Case study:** Ford battery researchers used InQuanto™ to study how quantum computers could be used to model lithium-ion batteries

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## ■ Introduction

As quantum computers mark new milestones on the path to scalable performance, the need for tools that fit into a modern technical workflow joins the priority list. Materials scientists, computational chemists, and other quantum professionals will need user-friendly tools to work with quantum computers, which will:

- Help them understand and explore today's quantum devices
- Integrate with their existing 'classical' workflows
- Easily experiment with different backends
- Take advantage of the rapidly growing corpus of quantum algorithms, embedding methods, and effective noise mitigation strategies.

Marwa H. Farag, a Ford quantum computer scientist, theoretical chemist and computational modeling expert, is the lead author on a new scientific paper that describes this approach to complex chemical modeling, "[Towards the simulation of transition-metal oxides of the cathode battery materials using VQE methods.](#)" Her colleague, Joydip Ghosh, is a physicist and the coauthor on this paper.

Marwa Farag and Joydip Ghosh are part of Ford's Core AI-ML-QC team lead by Devesh Upadhyay.



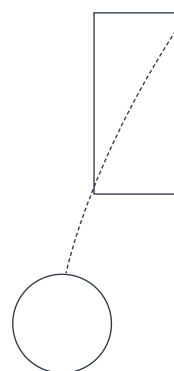
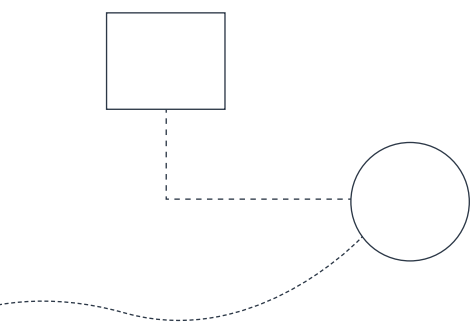
## ■ The challenge

**Quantum researchers at Ford Motor Company are seeking new ways to simulate the chemistry of lithium-ion batteries.**

Typically, highly accurate simulations of complex, real-world molecules are beyond the reach of the most advanced classical computers, due to the large size of the problem space, which grows exponentially with the size of the system. Quantum computers overcome this, with their computational power capable of scaling exponentially.

Farag & Ghosh researched lithium-ion battery chemistry using quantum computers. In this work, the scientists used the variational quantum eigensolver (VQE), an algorithm for finding the ground state of a quantum mechanical system. VQE is a hybrid quantum-classical algorithm, which is deployed on today's quantum computers to solve only the part of a molecular system that benefits most from the quantum computation, with the remaining calculations directed to a classical computer.

Using this hybrid approach, supported by Quantinuum's quantum chemistry platform InQuanto™, the team were able to work with molecules that are directly relevant to battery research. They also demonstrated a simulation that moves the field of quantum chemistry closer to being able to take on real-world problems on quantum computers.





## ■ User friendly for computational chemists

- **InQuanto is a software platform that can be used by chemists today to prepare for the quantum era.** Designed around the experimental workflow of a computational chemist, it provides researchers with everything they need to conduct efficient and effective quantum computational chemistry research.
- **By using InQuanto, a computational chemist can focus on the value-added element of their research.** Instead of writing a lot of code, a user can apply code and algorithms from the InQuanto library, which are already proven to be effective. Building new code from smaller building blocks also introduces the risk of errors
- **InQuanto provides comprehensive access to ansätze based on effective work in other projects and domains.** This speeds up the process of running experiments and supporting teams to target a wider range of potential outcomes relatively easily.
- **InQuanto is accessible for computational chemists who have and haven't worked with quantum systems before.** The platform is designed with an interface that is as easy to use for a computational chemist as possible. With InQuanto, the building blocks are in place, and they connect easily with existing computational workflows.
- **One key benefit of InQuanto is the automated circuit generation made possible by TKET, which is the foundation of the platform.** A user can write down a sequence of operations, but to compile it into a circuit that can be efficiently simulated, and the variational parameters optimized in finite time, may take a great deal of experience and is prone to failure. For example, if the depth is too high, you wouldn't be able to run the circuit at all.
- **The circuit compilation routines in InQuanto reduce circuit depth significantly.** This allows simulation of suitably scaled molecular and material problems on today's quantum hardware, including the IBM series of superconducting circuit devices, and Quantinuum's H Series of ion-trap devices, Powered by Honeywell, plus a range of other hardware devices and emulators.

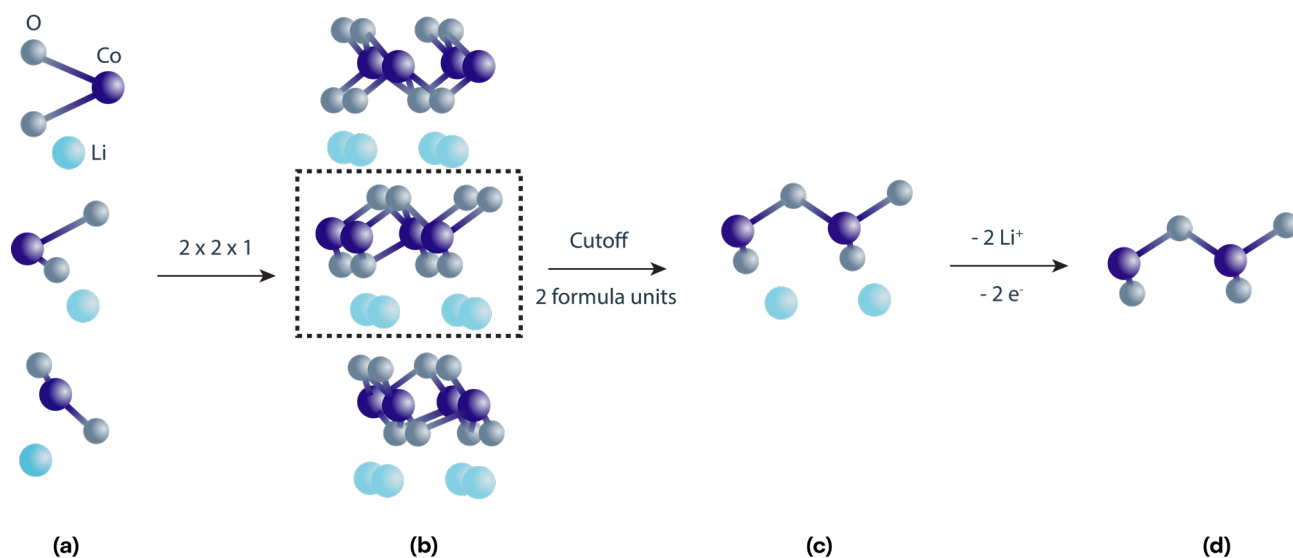


## ■ Solving a large and complex problem

Researchers at Ford first used InQuanto as part of the beta testing program in 2021. The company was a launch partner in May 2022 when the software was formally released.

Quantum computing is an emerging solution for a wide class of problems that are too challenging for existing high-performance computers. In the paper, the authors explain that accurate and universal tools are needed to simulate battery materials and guide the development of the next generation lithium-ion batteries, “in particular when the experimental results are unavailable.”

Figure 1: In Farag & Ghosh's experiment, a gas-phase model was used to mimic the building blocks of  $\text{LiCoO}_2/\text{CoO}_2$  for simulation on a quantum computer



## ■ How Farag & Ghosh's experiment worked

- Farag & Ghosh used a variational quantum eigensolver run in InQuanto to obtain the ground-state energy of  $\text{LiCoO}_2$ , a candidate transition metal oxide used for battery cathodes.
- They used a noiseless quantum simulator to create  $\text{Li}_2\text{Co}_2\text{O}_4$  and  $\text{Co}_2\text{O}_4$  gas-phase models, which represent the lithiated and delithiated states during the discharge and the charge of the Li-ion battery, respectively.
- The team demonstrated how the gas-phase model was defined to mimic the building block of the crystal structure of the material and how the active space is selected for the subsequent VQE simulations.
- The VQE simulations and computations yield calculated energies. Computations were performed using a state vector simulator with a single reference state for three different trial wavefunctions, finding that k-UpCCGSD (k-unitary pair coupled cluster generalized singles and doubles) produced the best results at a lower cost.
- The research team analyzed the required resources, including circuit depth, two-qubit entangling gates and wavefunction parameters. Benchmarking the performance of VQE methods against classical wavefunction-based methods, the team found that the results showed that VQE methods quantitatively agree with the results obtained from the classical methods.

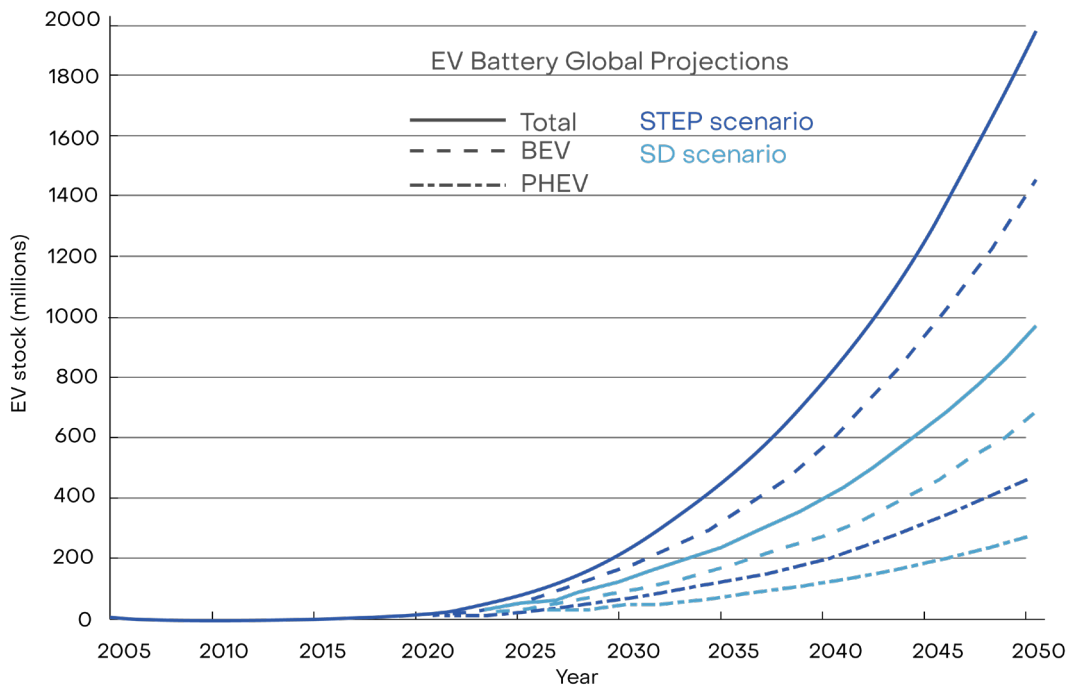
## ■ Meeting the demand for better batteries

By one estimate, the battery market will be worth \$100.4 billion by 2025<sup>1</sup>. Half of all those batteries will be used in electric vehicles. Lithium-ion batteries can be charged and discharged many times, but they also are sensitive to heat and inherently flammable.

Battery makers need to improve their product in many ways: energy density, power density, lifecycle, safety, cost, and recyclability. As the authors write in the paper, this is where quantum chemistry comes in.

“Computational chemistry can provide insights about the charge/discharge mechanisms, electrochemical and thermal stability, structural phase transition, and surface behavior, and it plays a vital role to find potential materials that can enhance the battery performance and robustness.” *Farag & Ghosh*

**Figure 2: Future battery electric vehicle (BEV) and plug-in hybrid electric vehicle (PHEV) projections, stated policy (STEP) and sustainable development (SD) scenarios<sup>2</sup>**



<sup>1</sup> "Ford Releases New Battery Capacity Plan, Raw Materials Details to Scale EVs" | Ford Media Center, July 21, 2022

<sup>2</sup> "Xu, C., Dai, Q., Gaines, L. et al. Future material demand for automotive lithium-based batteries. *Commun Mater* 1, 99 (2020). <https://doi.org/10.1038/s43246-020-00095-x>



## ■ Where next?

These experiments explored computations that are beyond what is possible on today's quantum computers. Quantinuum is rapidly improving the capabilities of its H-series hardware by:

- Scaling up qubit count
- Improving qubit quality
- Developing novel noise mitigation and error correction methods
- Pioneering the use of logical qubits
- Pioneering a flexible toolkit for developers including mid-circuit measurement, conditional logic, novel native gate sets, and techniques for qubit reuse

Quantinuum's quantum computational software platform InQuanto™ can expand what is possible on a wide range of near-term quantum hardware. InQuanto is platform inclusive, allowing chemists to direct their circuits to a dozen or more hardware or emulator back-ends.

### **Please contact**

[inquanto@quantinuum.com](mailto:inquanto@quantinuum.com)  
[www.quantinuum.com](http://www.quantinuum.com)

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