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# Accelerating Quantum Chemistry

## With Quantum Computers

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**Quantinuum** is the world's largest quantum computing company and, in collaboration with industrial partners, is accelerating quantum computational chemistry with quantum computers.

**Quantinuum InQuanto**, our proprietary state-of-the-art python platform, leverages our full stack and a range of quantum hardware to accelerate quantum computational chemistry research.

- ✓ **Up to 10x more accurate and resource efficient** than alternative open-source packages
- ✓ **Professionally developed and maintained code** with extensive documentation
- ✓ **Mix and match over 45** of the latest quantum algorithms and methods, including both variational and phase estimation algorithms
- ✓ **Customizable extensible workflow** for expert users down to the quantum circuit and hardware levels
- ✓ **Integrated with PySCF** to easily build hybrid quantum-classical workflows
- ✓ **Quantum error detection and correction** to enable logical qubits
- ✓ Compatible with **over 25 different quantum backends**, including a range of quantum hardware, simulators, emulators and cloud platforms

Transition State Characterization

Reaction Pathway Characterization

Catalysis

Solvation Methods

pKa Determination

Spectroscopic Properties

Molecular Mechanics

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**Classical Drivers & Embedding Methods**

**Variational Algorithms**

**Quantum Phase Estimation**

**Quantum Error Reduction Tools**

**Quantinuum Nexus:** Quantum workflow orchestration platform

**Open-source Quantinuum Software Libraries:** TKET | pytket | Qermit | phayes

**Quantinuum Systems**

**> 25 Third Party Platforms**

# What Can You Do
## With InQuanto?

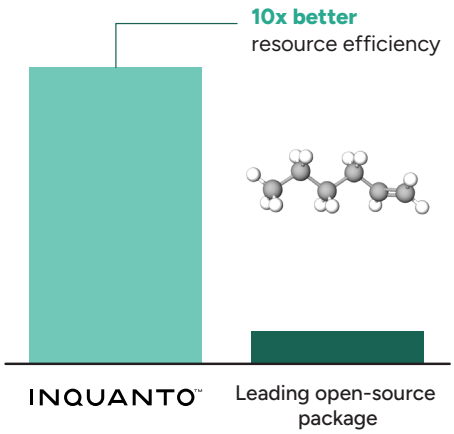
InQuanto enables **computational chemists** and **quantum researchers** who are exploring the capabilities of quantum computers to greatly improve the accuracy of complex molecular and materials simulations.

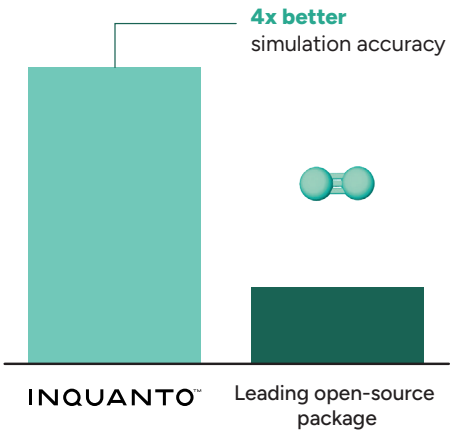
**Model industrially-relevant systems** using today's quantum hardware, leveraging InQuanto's embedding methods (DMET, QM/MM, FMO, WFT-in-DFT), and chemistry-specific noise mitigation and circuit synthesis techniques to optimize performance across various backends

**Develop new methods** with InQuanto's modifiable and extensible workflow, that includes a number of fully customizable classes, a range of ansatzes and solvers, low level methods down to the quantum circuit and hardware, and resource estimation tools for phase estimation algorithms

**Educate your team** with professionally developed and maintained code, extensive documentation and tutorials, support from our expert team and custom webinars and technical workshops

InQuanto **consistently outperforms** leading open-source packages in terms of resource efficiency and simulation accuracy.



# Published Studies

## With Our Collaborators Using InQuanto

### Quantifying $CO_2$ Binding in Metal Organic Frameworks using Density Matrix Embedding with **TotalEnergies**

Performed an embedded simulation of aluminum - $CO_2$ bond in a metal organic framework to prototype accurate simulations of complex bonds in large systems.

### Quantum Computational Quantification of Protein-Ligand Interactions with **Roche** pRED

This is the first demonstration of the quantification of drug-protein interactions on quantum computers, through a quantum simulation embedded in a 20k-atom QM/MM scheme.

### Modeling Transition-metal Oxides of the Cathode Battery Materials Using Quantum Computing Methods with **Ford Motor Company**

Ford Motor Company simulated the ground state of $LiCoO_2$ using InQuanto and its PySCF interface for classical pre-processing.

### Modeling the Oxygen Reduction Reaction in Hydrogen Fuel Cells with **Airbus** and **BMW Group**

Modeled the Oxygen Reduction Reaction on a Pt and Pt/Co catalyst using a workflow developed in InQuanto and implemented on our H1-1 trapped-ion quantum computer.

### Studying a Reaction in Atomic Layer Deposition with **Air Liquide**

Developed new protocol to simulate the atomic layer deposition of a zirconium precursor on a hydroxylated silicon surface.

### Modeling the Absorption Spectrum of Methane and its Reaction with an Atmospheric Radical with **Honeywell Advanced Materials**

Used a new state-preparation method, now in InQuanto, with noise mitigation to perform one of the largest excited state calculations to date, and simulate an atmospheric reaction on a quantum computer for the first time.

### Quantum Hardware Calculations of the Activation and Dissociation of $N_2$ on Iron Clusters and Surfaces with **Equinor**

Developed a prototype hybrid quantum-classical workflow using InQuanto for modeling chemical reactions on surfaces.

# What's New
## in InQuanto

1 **Replicate and build upon our recent breakthrough paper**[1] demonstrating quantum phase estimation with quantum error correction using our System Model H2. See our new Knowledge Article at **docs.quantinuum.com/inquanto/tutorials/InQ_KA_h2xh2.html** to learn more.

2 **Interface with NVIDIA's CuTensorNet Library**

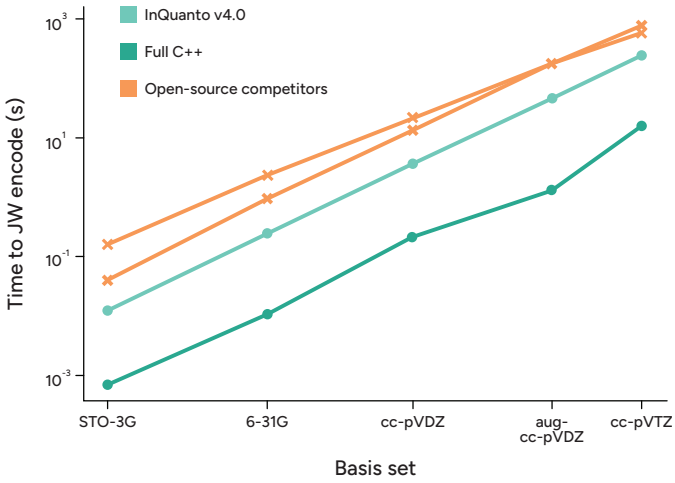
InQuanto is now interfaced with NVIDIA's high performance cuTensorNet library via our pytket-cutensornet extension, which unlocks large-scale and high-precision quantum simulations for InQuanto users with GPU access.

3 **Integration with Quantinuum Nexus**

InQuanto is now integrated with Quantinuum Nexus, our comprehensive quantum computing cloud platform. Users will benefit from zero-set up access to InQuanto and can leverage all of Nexus features in their workflows, including easy data storage, access to Quantinuum System emulators, collaboration tools, and much more...

4 **Enhanced Operator Performance**

InQuanto v4.0 integrates C++ implementations of the operator classes within the mappings module, yielding significant gains in performance. InQuanto users will not experience any change in their interaction with the mappings module or the operator classes but will benefit from a classical pre-processing speed-up.




Performance comparison of Jordan Wigner (JW) operator mappings for LiH molecule in different basis sets.

1. https://arxiv.org/abs/2505.09133

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# Next Steps →

Please reach out to us at **quantinuum.com/connect** to learn more about InQuanto, or contact **Simon McAdams**, Quantum Chemistry Product Lead, at **inquanto@quantinuum.com.**

## About Us

Quantinuum, the world's largest integrated quantum company, pioneers powerful quantum computers and advanced software solutions. Quantinuum's technology drives breakthroughs in materials discovery, cybersecurity, and next-gen quantum AI. With over 630 employees, including 440+ scientists and engineers, Quantinuum leads the quantum computing revolution across continents.

For more information, please visit **quantinuum.com.**

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See our InQuanto documentation at
**docs.quantinuum.com**