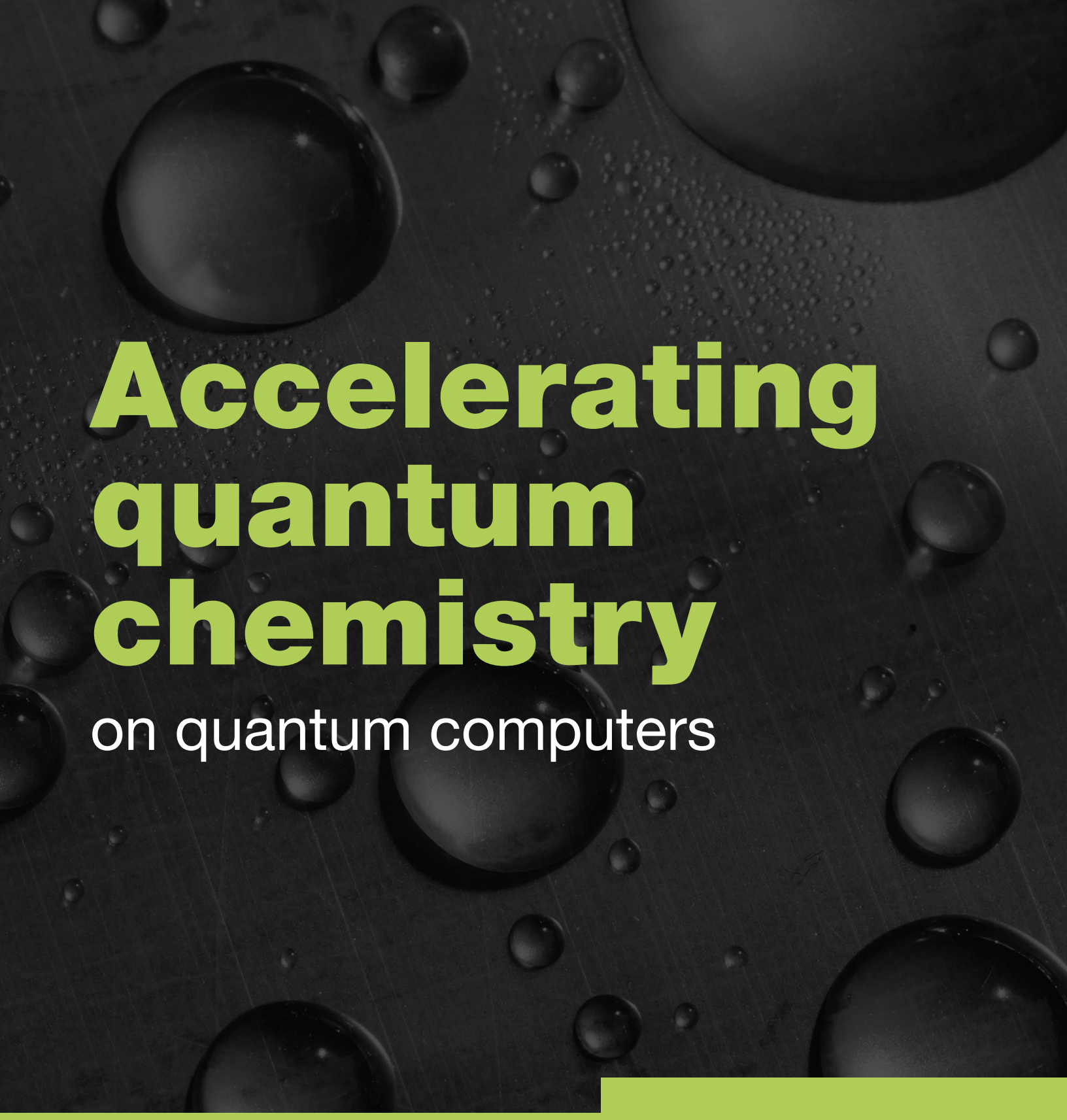


Accelerating quantum chemistry

on quantum computers

INQUANTO™
v3.0

QUANTINUUM

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

Quantinuum has developed **InQuanto**™, a state-of-the-art python platform that 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 leading open-source competitors
- ✓ **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 and extensible workflow** for expert users down to the quantum circuit and hardware levels
- ✓ **Integrated with PySCF** to easily build hybird-classical quantum workflows
- ✓ **Proprietary quantum error detection & chemistry-specific noise mitigation** to reduce resources and enable logically-encoded qubits
- ✓ Compatible with **over 25 different quantum backends**, including a range of quantum hardware, simulators, emulators and cloud platforms
- ✓ Unique access to our **H-Series hardware & emulators**, the world's most powerful quantum computers

Transition State Characterization

Reaction Pathway Characterization

Catalysis

Solvation Methods

pKa Determination

Spectroscopic Properties

Molecular Mechanics

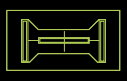
INQUANTO™

Classical Drivers & Embedding Methods

Variational Algorithms | **Quantum Phase Estimation**

Quantum Error Detection & Noise Mitigation

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



H-Series Quantum Computers
Powered by **Honeywell**

> 25 Third Party Platforms

What can you do
with InQuanto?

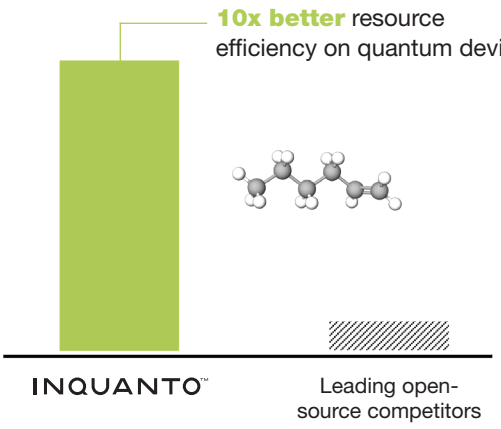
InQuanto enables **computational chemists** and **quantum researchers** who are exploring the capabilities of quantum computers to greatly improve the accuracy of complex molecular and materials simulations.

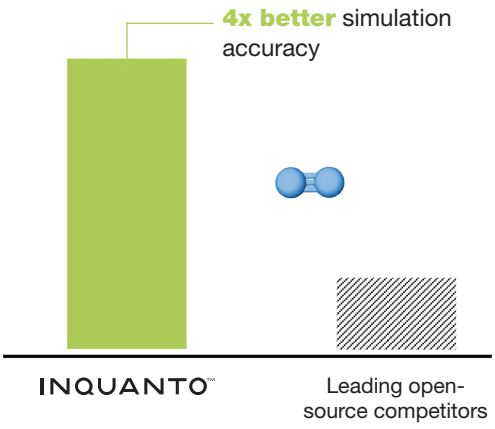
Model industrially-relevant systems using today's quantum hardware, leveraging InQuanto's embedding methods (DMET, QM/MM, FMO, WFT-in-DFT), and chemistry-specific noise mitigation and circuit synthesis techniques to optimize performance across various backends

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 levels, 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 on a range of quantum backends.





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.

Quantum Hardware Calculations of Solid-state Iron Crystals

This was the first demonstration of periodic UCC calculation on a quantum device where we developed a novel noise mitigation technique called measurement symmetry verification, now available in InQuanto.

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.

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 the first-time atmospheric reaction simulated on a quantum computer.

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.

Modeling Transition-metal Oxides of the Cathode Battery Materials Using Quantum Computing Methods

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

What's new
in InQuanto v3.0

1 Quantum Phase Estimation Algorithms

With variational quantum algorithms reaching today's practical limits, InQuanto now offers a range of stochastic and deterministic quantum phase estimation (QPE) algorithms, including:

- Basic canonical QPE
- Iterative QPE
- Information theory QPE
- Kitaev's QPE
- Bayesian QPE

Which now include resource estimation tools:

- Users can input a chemical system and check how deep and wide the quantum circuits will be, and how they are optimized with pytket
- For stochastic QPEs, users can further estimate how many shots are needed, and how effective noise mitigation techniques are when simulating the systems of interest using Quantinuum's emulator

2 Quantum Error Detection and Qermit Integration

Quantinuum's proprietary quantum error detection code, which enabled the first demonstration of QPE on error detected logical qubits is now available in InQuanto v3.0.

- Users can now mix and match both QPE and VQE algorithms with the QED code, and interface with Quantinuum's open-source python package for noise mitigation, Qermit, to improve quantum hardware results and experiment with logically-encoded qubits

3 Green's Functions

- Our recent paper *(https://arxiv.org/abs/2309.09685)* applied the Lanczos cumulant expansion as an advanced excited state method for quantum computed Green's Function quantities
- The method avoids high number of measurements associated with previous VQE-based methods
- InQuanto v3.0 now enables Green's Function quantities to be calculated on quantum hardware, noisy simulators, and statevector simulators

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 almost 500 employees, including 370+ scientists and engineers, Quantinuum leads the quantum computing revolution across continents.

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

Learn more about
INQUANTO™

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