



Quantum Computational  
Chemistry Platform for  
Quantum Computers

**INQUANTO™**



## ■ WHY QUANTUM COMPUTING?

Quantum chemistry aims to accurately describe and predict the fundamental properties of matter, and hence is a powerful tool in the design and development of new molecules and materials. However, molecules and materials of industrial relevance are complex and not easy to accurately simulate. Today's capabilities force a trade to either use highly accurate methods on the smallest sized systems or use approximating techniques. The former is not large enough to be of relevance and the latter is not accurate enough to disrupt today's development life cycle.

The future of quantum computing poses an interesting capability: the potential to make highly accurate calculations of industrial relevant molecules efficiently implemented for the computational chemist.

## ■ LEVERAGING THE POWER OF QUANTUM COMPUTING TODAY

With the quantum computers available today, scientists are starting to simulate simple systems, which are gradually increasing in complexity as quantum computers develop.

But how can you leverage today's quantum computers to go beyond these simple systems and simulate industrially relevant molecules and materials?

Quantinuum has developed InQuanto™, a state-of-the-art quantum computational chemistry platform, that enables computational chemists to easily experiment with a wide range of algorithms on today's devices for their real-world use cases.

InQuanto, now available for the first time as a standalone platform for organisations, brings together the latest quantum computing tools in a single application.

## ■ REAL WORLD USE CASES ON REAL QUANTUM COMPUTERS

InQuanto's modular workflow enables both computational chemists and quantum algorithm developers to easily mix and match the latest quantum algorithms with advanced subroutines and error mitigation techniques to get the best out of today's quantum platforms.

With InQuanto, users have access to unparalleled customisation and control of their quantum chemistry experiments. They can leverage advanced qubit encoding and embedding techniques to reduce resource requirements to unlock the modelling of larger systems than ever before, using today's quantum devices.

“Nature isn't classical, if you want to make a simulation of nature, you'd better make it quantum mechanical.”

Professor Richard Feynman  
*Theoretical Physicist*

## ■ INQUANTO FEATURES

### USABILITY

Easy to build and execute experiments in one ecosystem.

### LATEST ALGORITHMS

Choose from the latest quantum algorithms and subroutines.

### FLEXIBILITY

Develop and run your own algorithms within InQuanto.

### SCALABILITY

Advanced qubit encoding and embedding to reduce resource requirements.

### NOISE MITIGATION

Leverage novel and chemistry-specific noise-mitigation techniques.

### CUSTOMISATION

Entry and exit points to analyse and customise experiments.

### CONTROL

End-to-end manipulation from classical to quantum and back.

### MULTIPLE BACKENDS

Choose from the largest number of quantum devices and simulators.

### COMPATIBILITY

InQuanto is compatible with Mac, Linux and WSL operating systems.



Ground & Excited  
State Energy Calcs




Spectroscopic  
Properties



Molecular  
Docking




Binding  
Affinity




pKa  
Determination



Transition  
States



Reaction  
Pathways



Solvation  
Models

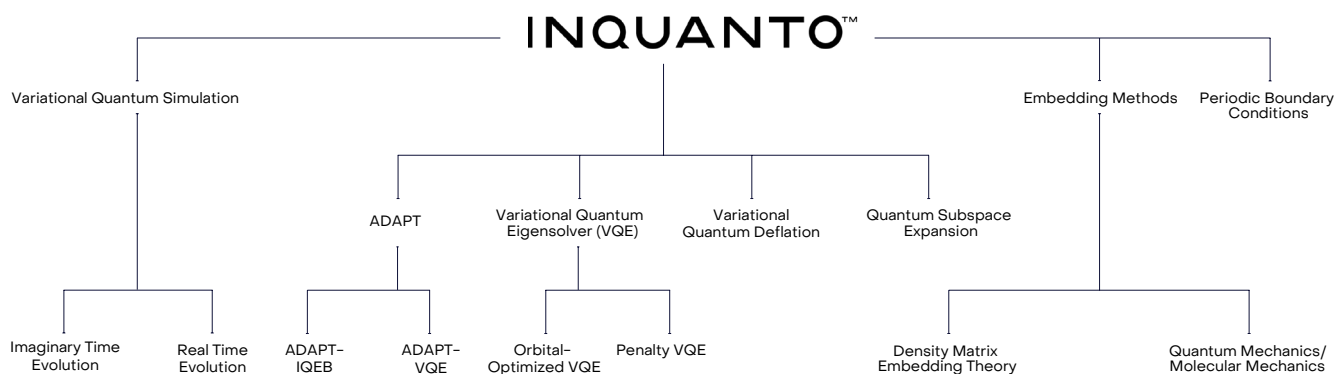


Crystal Structure  
Determination



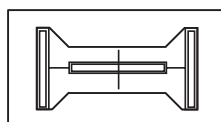
Molecular  
Mechanics

## MOLECULE/MATERIAL



## TKET - QUANTUM SOFTWARE DEVELOPMENT PLATFORM

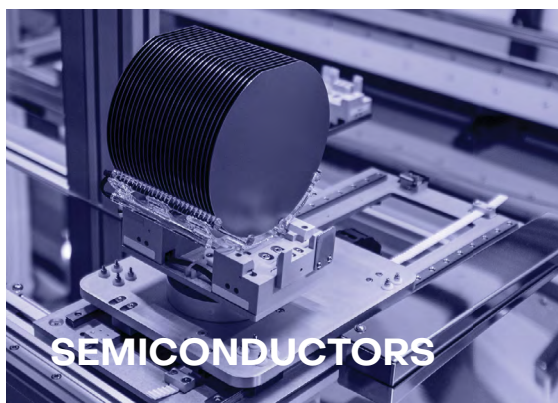
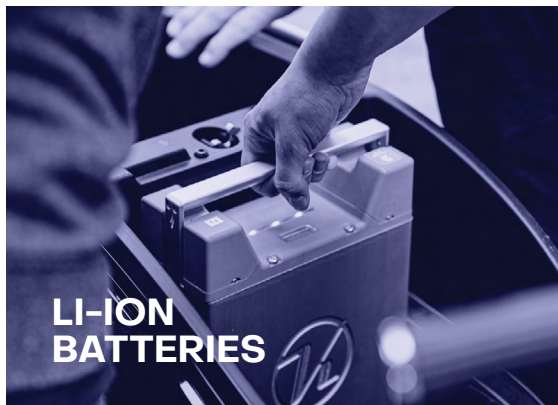
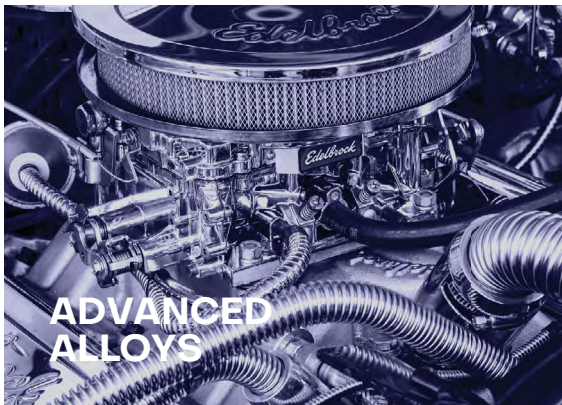
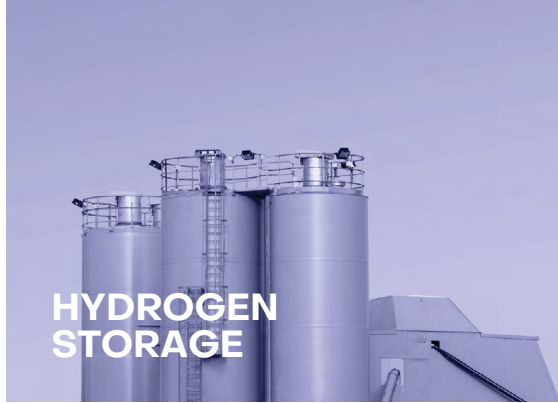
Other Quantum  
Computer Processors



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

## ■ APPLICATION AREAS

InQuanto was developed and deployed by Quantinuum's quantum chemistry team. It supports collaborations with industrial partners exploring quantum computing use cases from drug design to next-generation materials. It is now available in a stand-alone software platform for use in a wide range of application areas.



## ■ INQUANTO INDUSTRIAL COLLABORATIONS

### MANUFACTURING

A Top 5 Steel Manufacturer  
Simulating Solid-state Iron Crystals

InQuanto has enabled the development and deployment of quantum algorithms for simulating crystalline materials on today's devices using advanced noise mitigation techniques.

[See our paper "Quantum Hardware Calculations of Periodic Systems: Hydrogen Chain and Iron Crystals."](#)

### PHARMACEUTICAL

A Top 5 Pharmaceutical Company  
Quantifying Drug-protein Interactions

InQuanto enables users to simulate the binding affinities of small molecule drugs to target proteins using today's devices.

[See our paper "Quantum Computational Quantification of Protein-Ligand Interactions."](#)

### ENERGY

A Top 5 Energy Company  
Metal-Organic Frameworks (MOFs) for Carbon Capture and Storage

InQuanto's embedding and fragmentation techniques enabled the modeling of CO<sub>2</sub> binding in an MOF for the first time using today's quantum computing resources.

[See our paper "Modelling Carbon Capture on Metal-Organic Frameworks with Quantum Computing."](#)

## ■ WHY GET STARTED WITH QUANTINUUM AND INQUANTO TODAY?

- Identify use cases amenable to quantum computing.
- Assess the capabilities of today's quantum computers and estimate resource requirements.
- Educate and enable your workforce in quantum computing methodologies and InQuanto.
- Start to integrate quantum computing into your existing workflows.

## ■ CONTACT US

Please contact our team at  
Email: [InQuanto@quantinum.com](mailto:InQuanto@quantinum.com)

[LinkedIn](#)  
[Quantinum.com](#)