Microsoft

Accelerating Computational Chemistry and Materials Science Research with Azure Quantum Elements

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96% of all manufactured goods rely
on chemicals and chemical manufacturers

A R&D paradigm shift is emerging with computation as an equal partner

Legacy

Wet lab

Explanatory modeling

Emerging

Empowering your R&D teams for your next breakthrough

Help identify better candidates faster and accelerate your innovation cycle

AZURE QUANTUM

Elements

Accelerating scientific discovery

Scale

- **Unbounded** exploration
- Screen **30,000,000** candidates in the same timeframe as **1,000**

Speed

- Expand **research horizons**
- Accelerate modeling of certain chemical processes by **500,000x**

Accuracy

- Solve **complex challenges** accurately
- Enable **predictive chemical design** up to **100x** accuracy

Bringing product to market faster

Enabling a faster innovation cycle with Copilot in Azure Quantum

Copilot in Azure Quantum

Harness the power of AI assistance within your cloud environment to improve research efficiency.

Large language models for ease of use

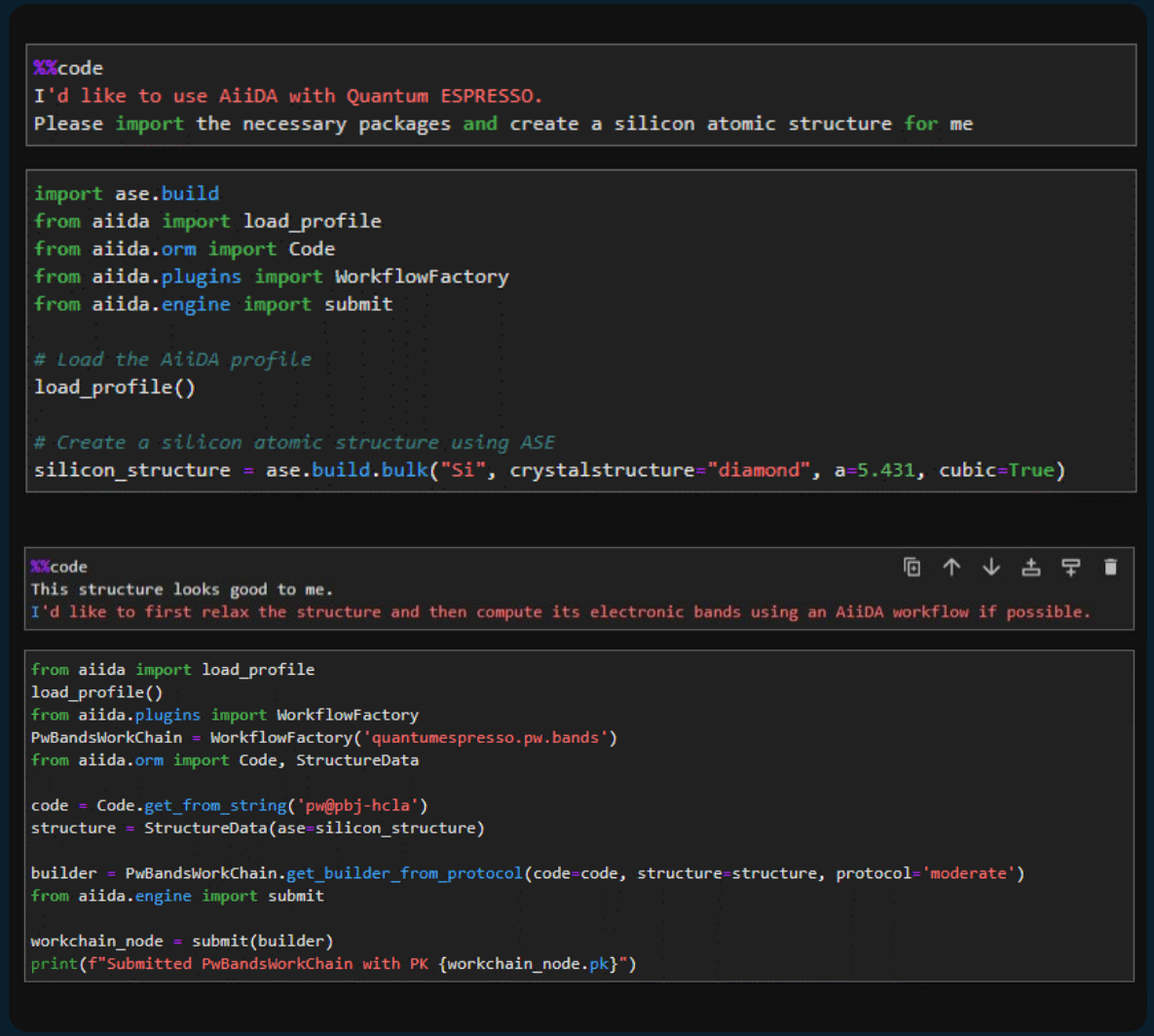
- Faster R&D innovation cycle
- Research efficiency with an AI agent integrated in your virtual environment

Custom applications

- Integrate conversational interface with PubChem and other databases
- Code generation for new and existing workflows

Resource: Chemistry Copilot in Azure Quantum:

➢ https://quantum.microsoft.com/en-us/experience/quantum-elements



Scale

High-performance computing

Scale with HPC automation

Scale | Speed | Accuracy

Elastic compute | Cloud-optimized | Cloud burst

Purpose-built HPC

Fast, Secure Networking

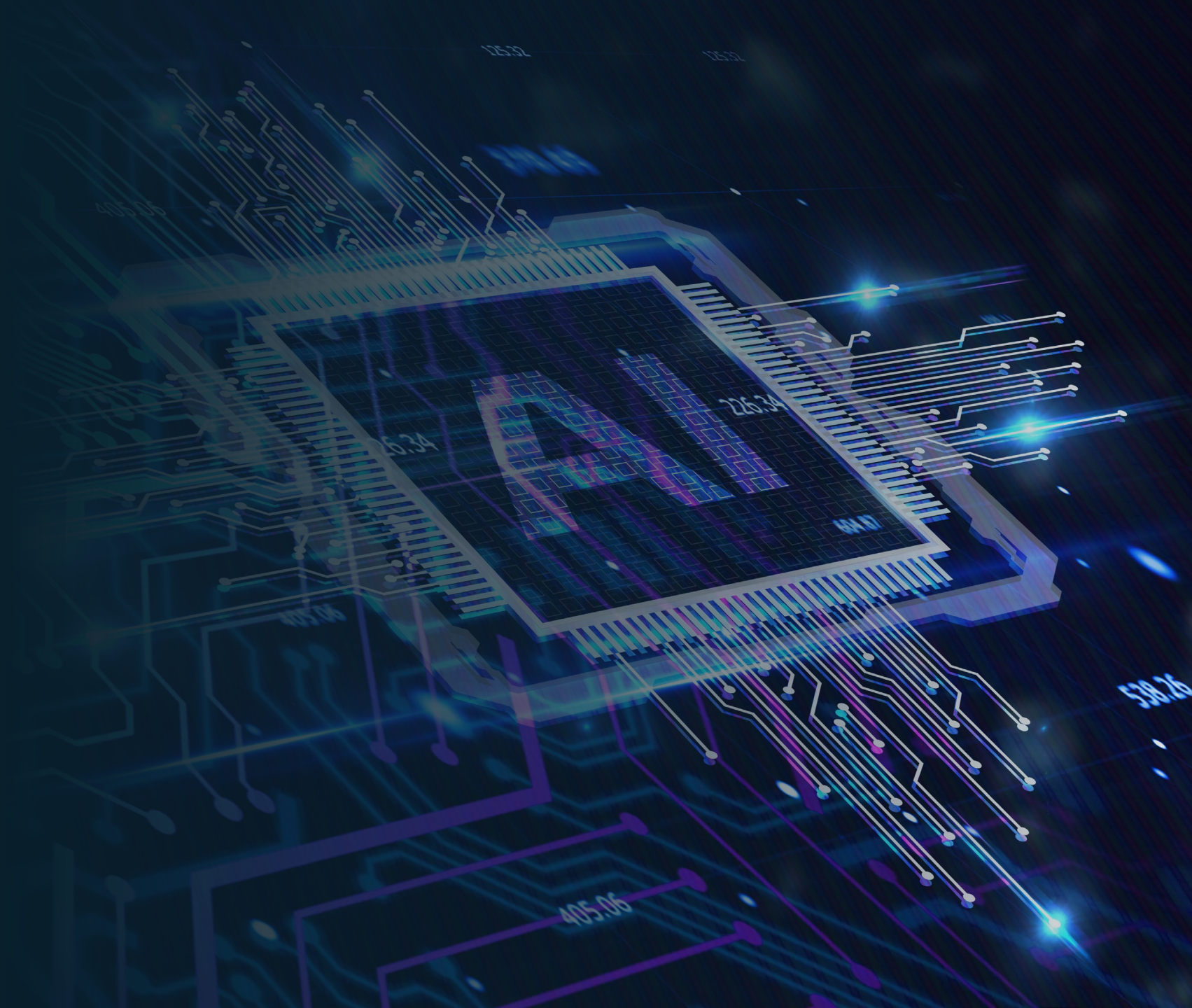
High Performing Storage

Workload Orchestration

Azure scale

Speed

Artificial Intelligence

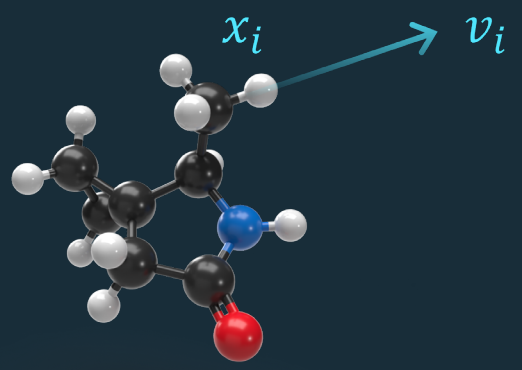


Speed with Artificial Intelligence

Scale | Speed | Accuracy

Train using simulations

First principles simulator

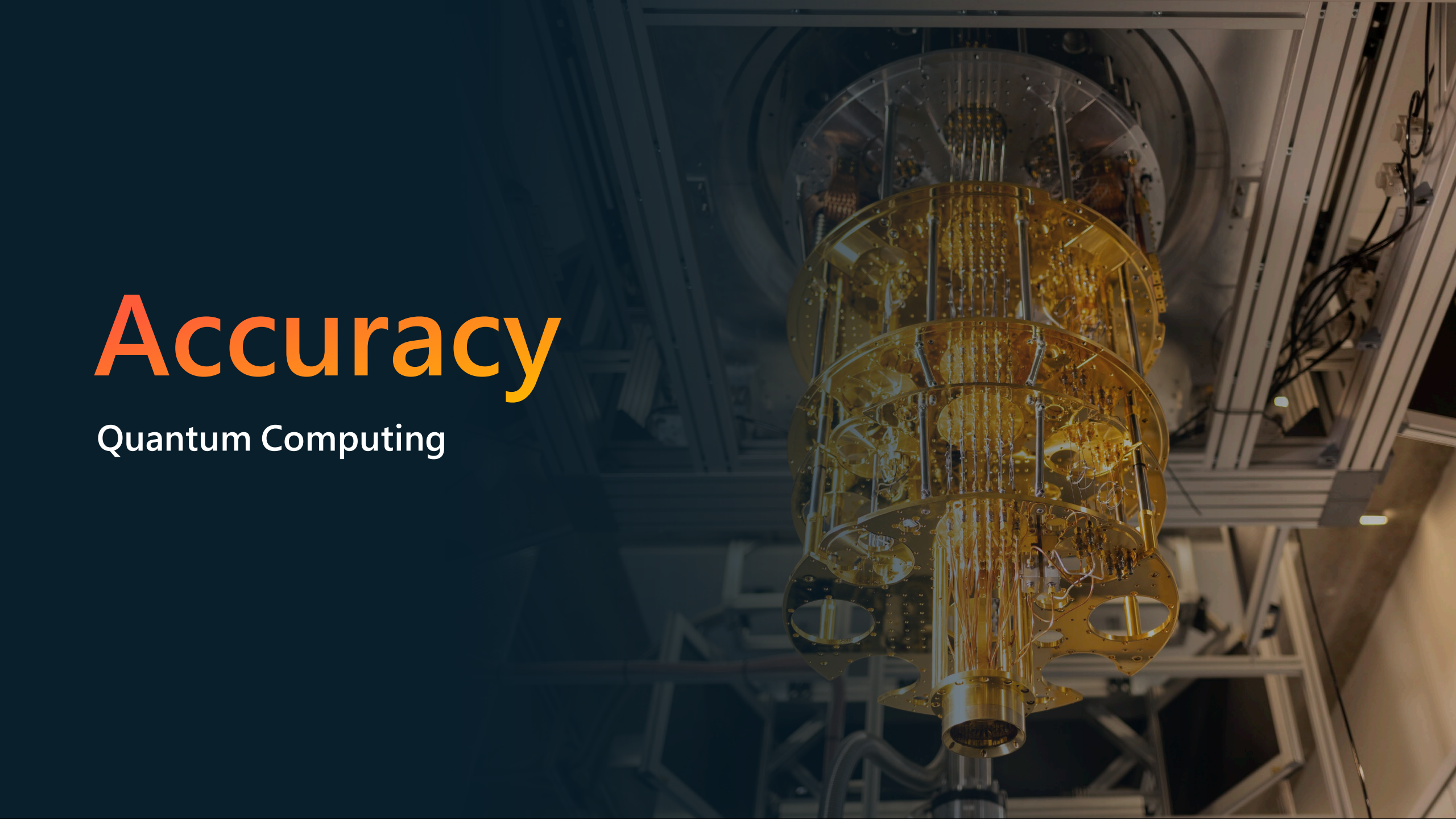


AI emulator

Simulate faster

Accuracy

Quantum Computing



Estimating quantum computing needs for accurate calculations

PASQAL

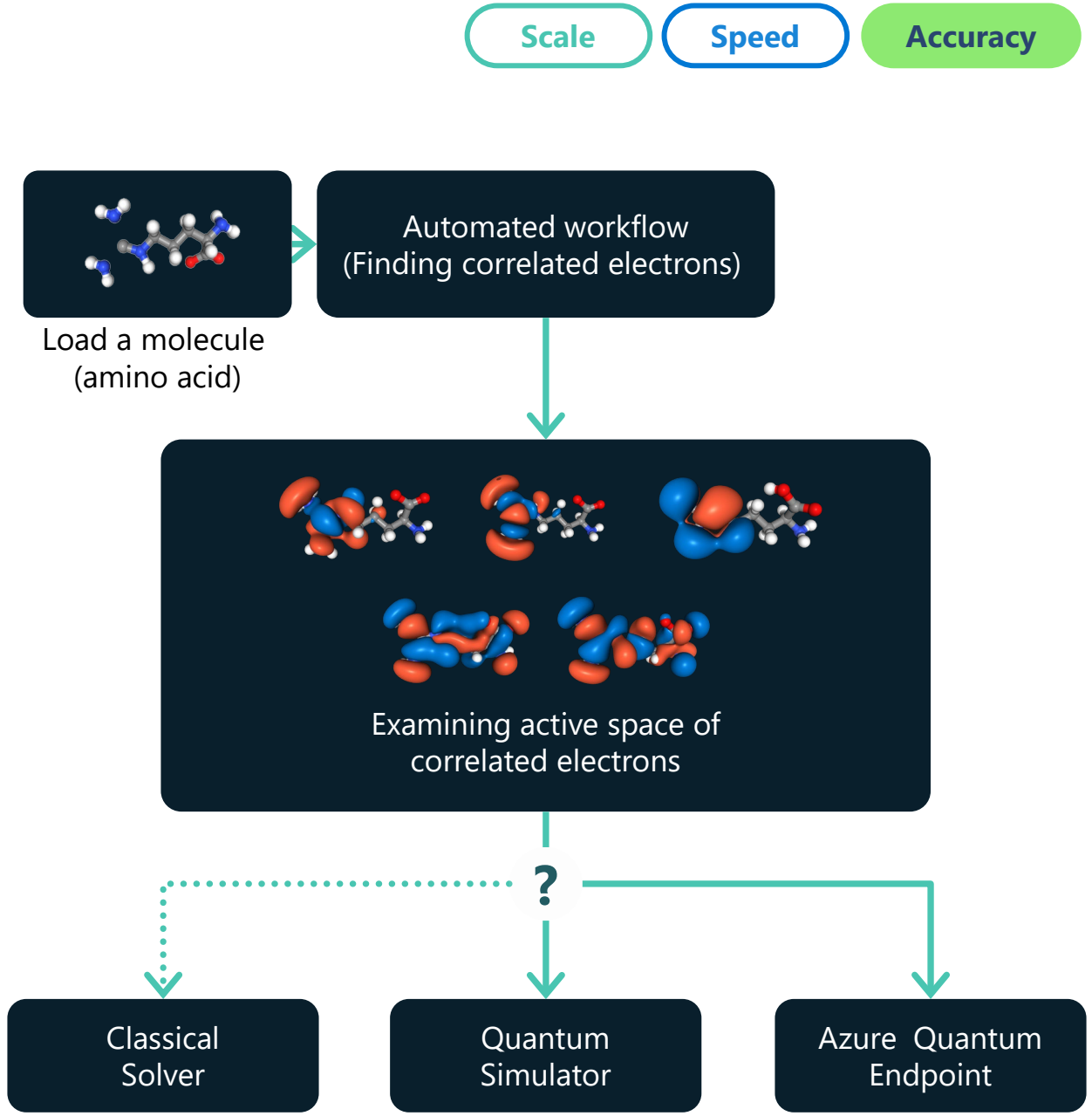
IONQ

QUANTINUUM

qci

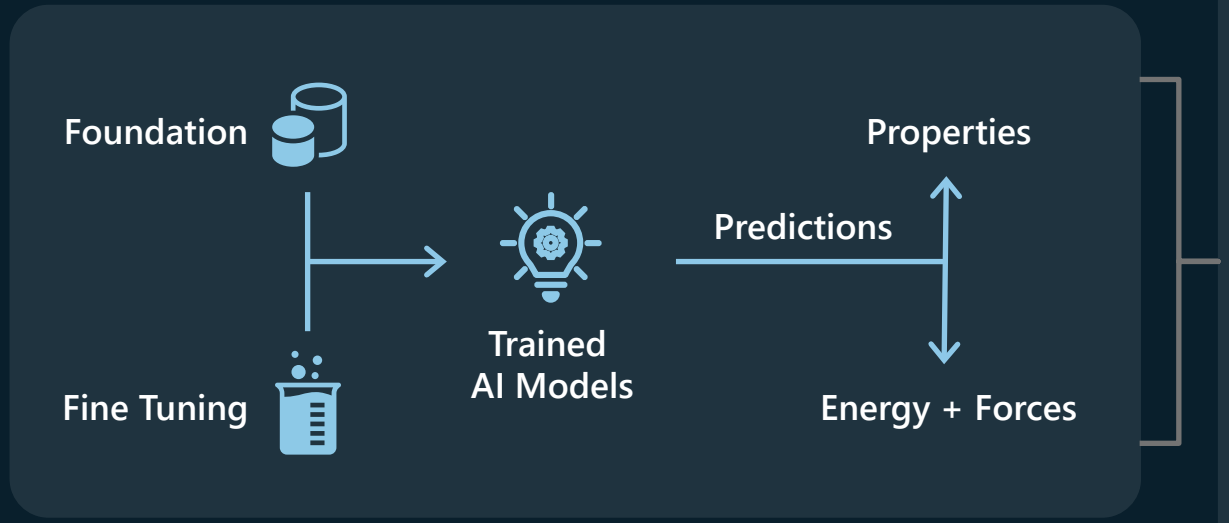
rigetti

Publication: Tomesh et al., "Optimized Quantum Program Execution Ordering to Mitigate Errors in Simulations of Quantum Systems," 6th IEEE International Conference on Rebooting Computing (2021).

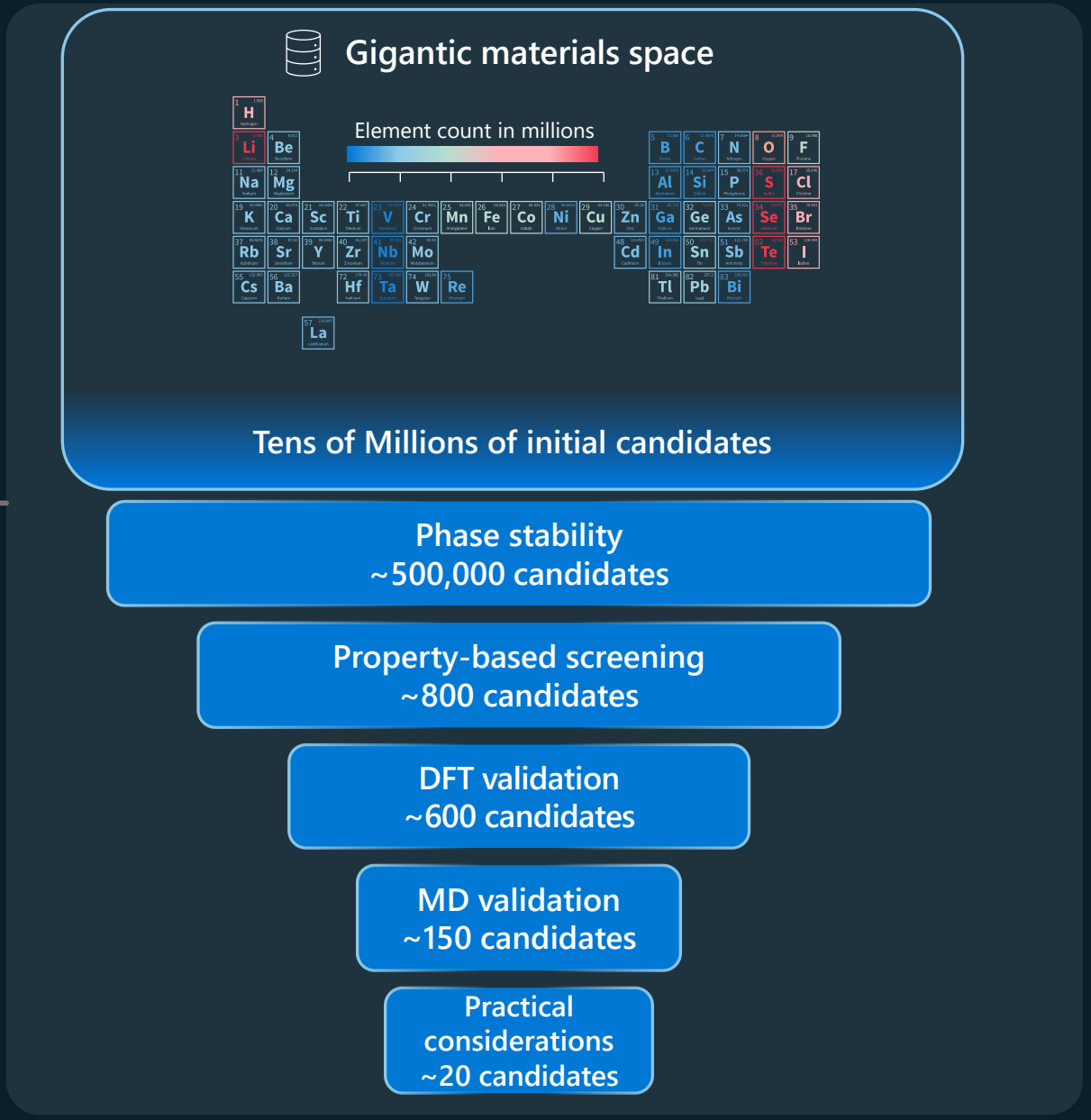


Accelerating chemical and materials discovery with AI Services

Compressing hours to seconds in simulation time



- **AI models**
  Trained on hundreds of thousands to millions of chemistry and materials data
- **Fine-tuning application**
  Predict solubility, boiling point, bioactivity, band gaps, spectroscopy ….



From 1K to 30M initial candidates (30,000x search space)

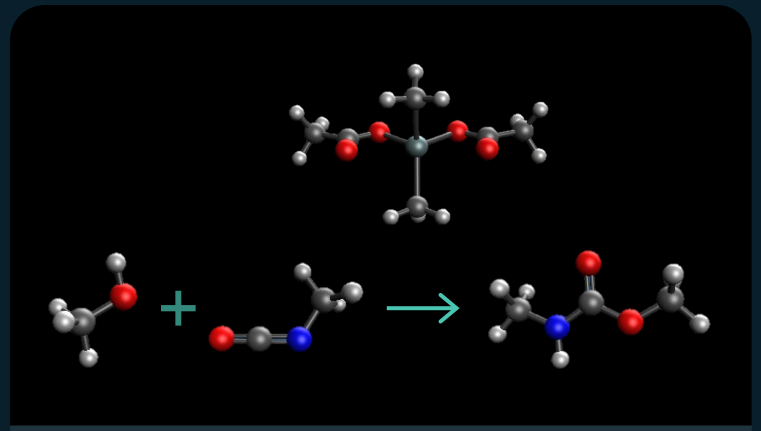
CUSTOMER STORY

Reaction network exploration with the scale of Azure

Understanding a long-standing controversy in homogeneous catalysis of urethane

Foundation of poly-urethane (PU) industry:

- 25M tons/year, 6% of world's total polymer production
- The catalyst studied has been used in industry for 4 decades without fully understanding the mechanism
- With the scale of Azure, we evaluated 1.5M+ reactions, clarified key mechanism and identified opportunities to improve the catalyst



"Truly impressive!
No one in the world has ever done such a study before."

Customer feedback

Optimized coupled-cluster calculations

Publication: Unsleber et al., "High-throughput ab initio reaction mechanism exploration in the cloud with automated multi-reference validation," J. Chem. Phys. 158, 084803 (2023).

Microsoft

We invite you to join us on this journey.

Register to learn more about the **Azure Quantum Elements preview**

Visit the **Azure Quantum Elements site**

Watch the **Quantum Innovator Webinar series.**