

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>

```
%%code
I'd like to use AiiDA with Quantum ESPRESSO.
Please import the necessary packages and create a silicon atomic structure for me
```

```
import ase.build
from aiida import load_profile
from aiida.orm import Code
from aiida.plugins import WorkflowFactory
from aiida.engine import submit

# Load the AiiDA profile
load_profile()

# Create a silicon atomic structure using ASE
silicon_structure = ase.build.bulk("Si", crystalstructure="diamond", a=5.431, cubic=True)
```

```
%%code
This structure looks good to me.
I'd like to first relax the structure and then compute its electronic bands using an AiiDA workflow if possible.
```

```
from aiida import load_profile
load_profile()
from aiida.plugins import WorkflowFactory
PwBandsWorkChain = WorkflowFactory('quantumespresso.pw.bands')
from aiida.orm import Code, StructureData

code = Code.get_from_string('pw@pbj-hcl1a')
structure = StructureData(ase=silicon_structure)

builder = PwBandsWorkChain.get_builder_from_protocol(code=code, structure=structure, protocol='moderate')
from aiida.engine import submit

workchain_node = submit(builder)
print(f"Submitted PwBandsWorkChain with PK {workchain_node.pk}")
```



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

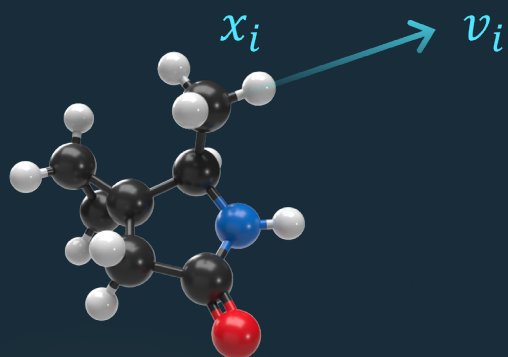
Scale

Speed

Accuracy

Train using simulations

First principles simulator



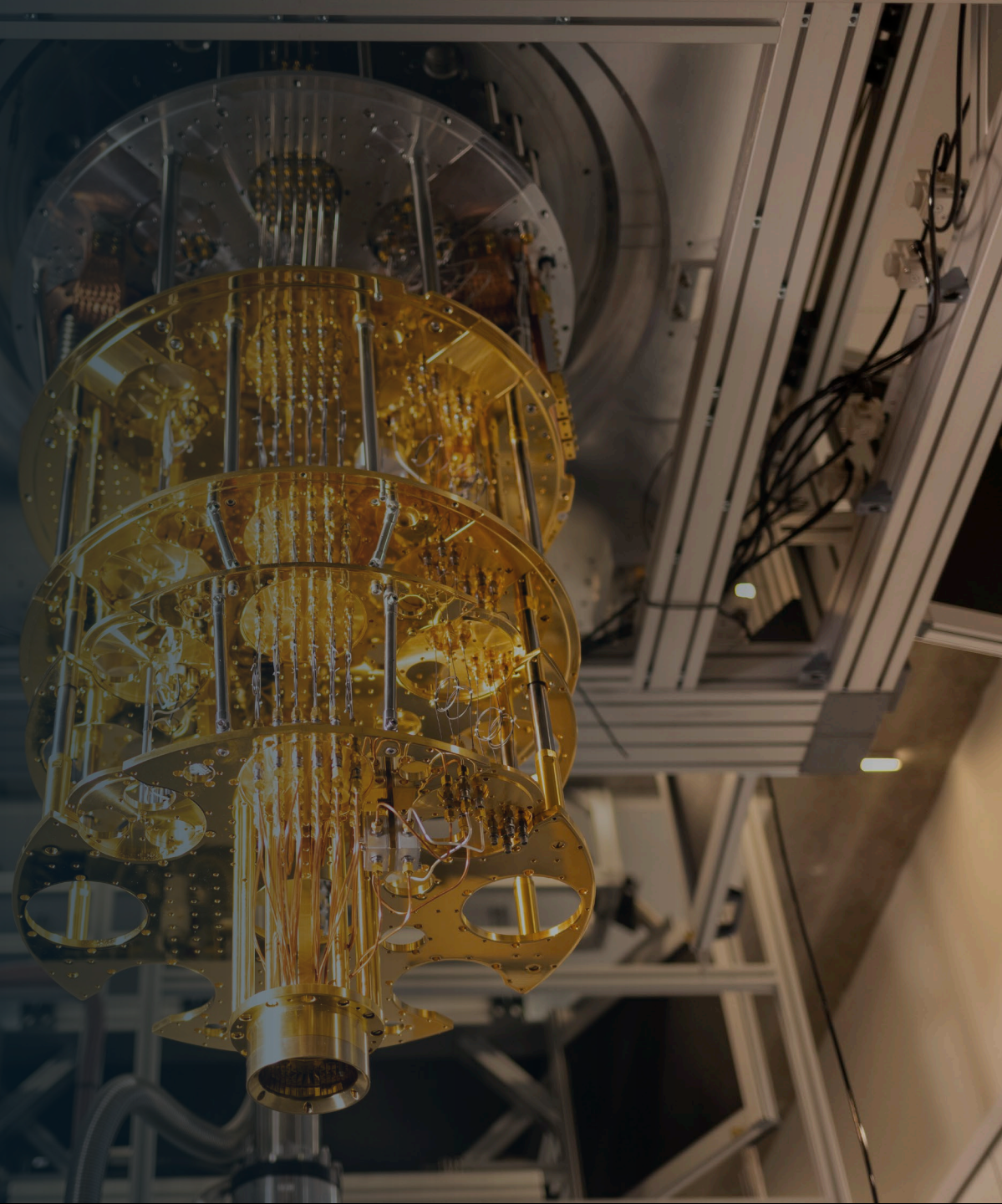
Simulate faster

AI emulator



Accuracy

Quantum Computing



Estimating quantum computing needs for accurate calculations

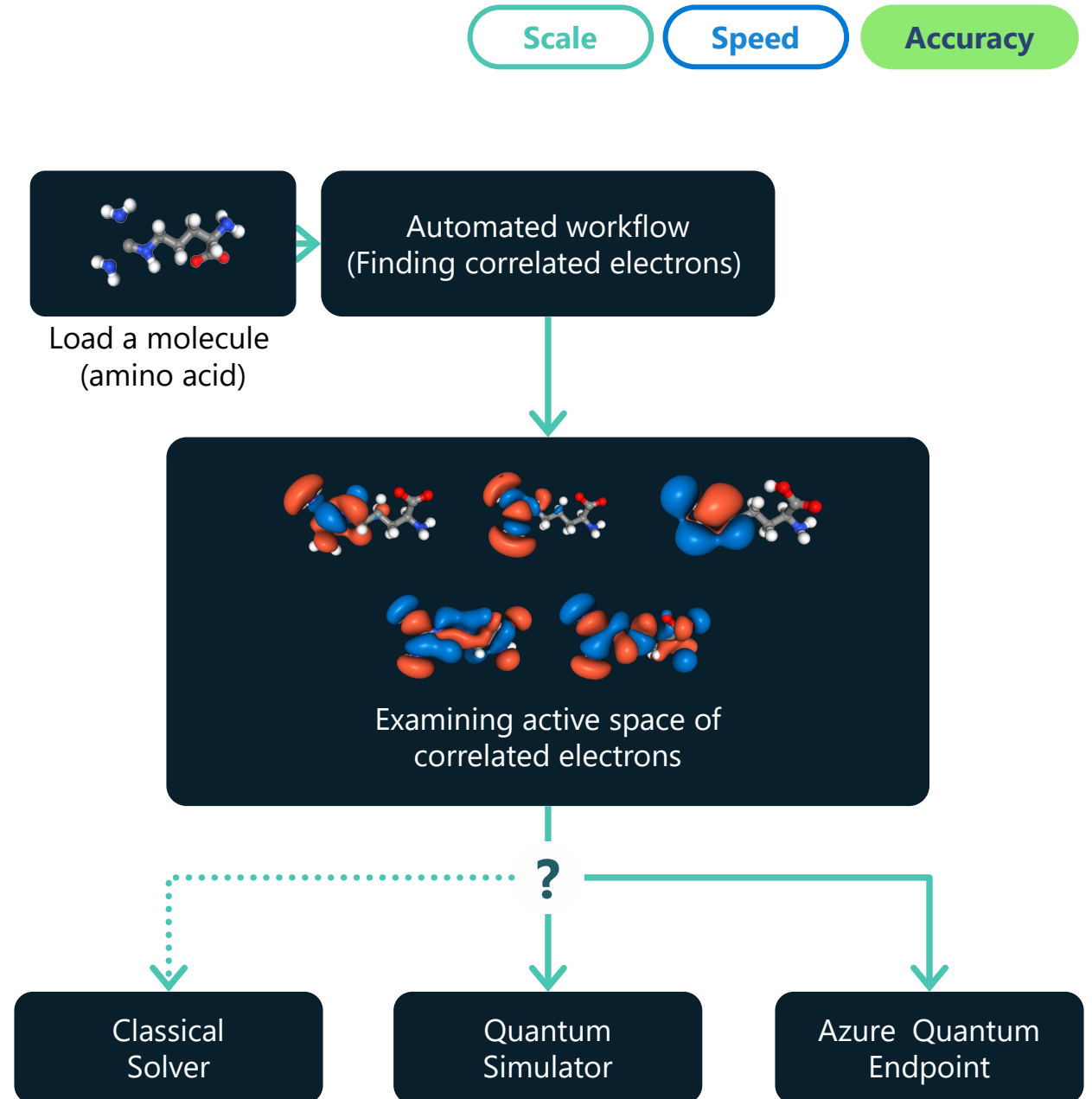


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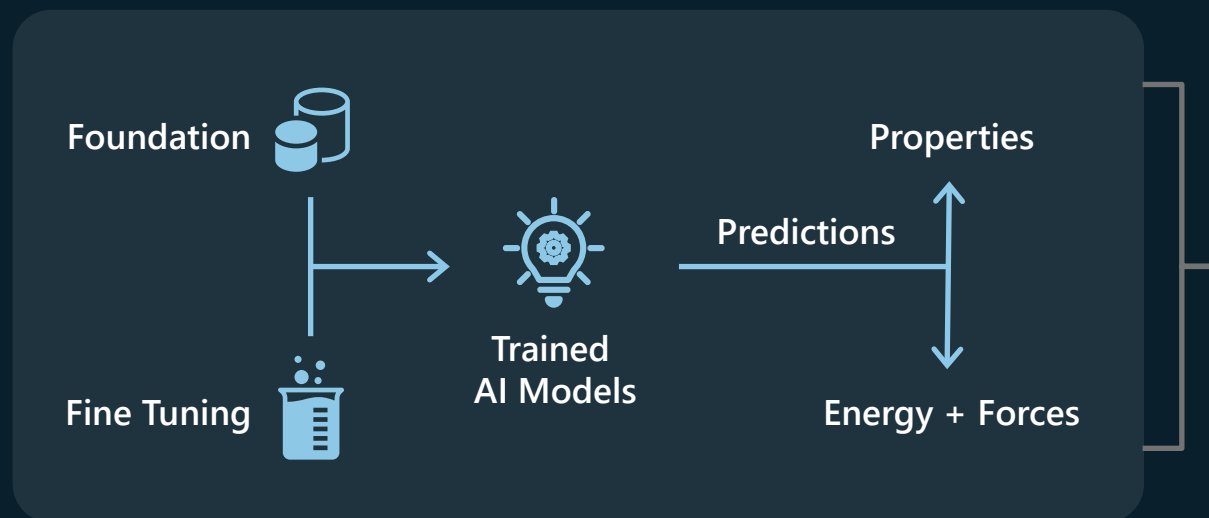
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Publication: Tomesh et al., "Optimized Quantum Program Execution Ordering to Mitigate Errors in Simulations of Quantum Systems," 6th IEEE International Conference on Rebooting Computing (2021).

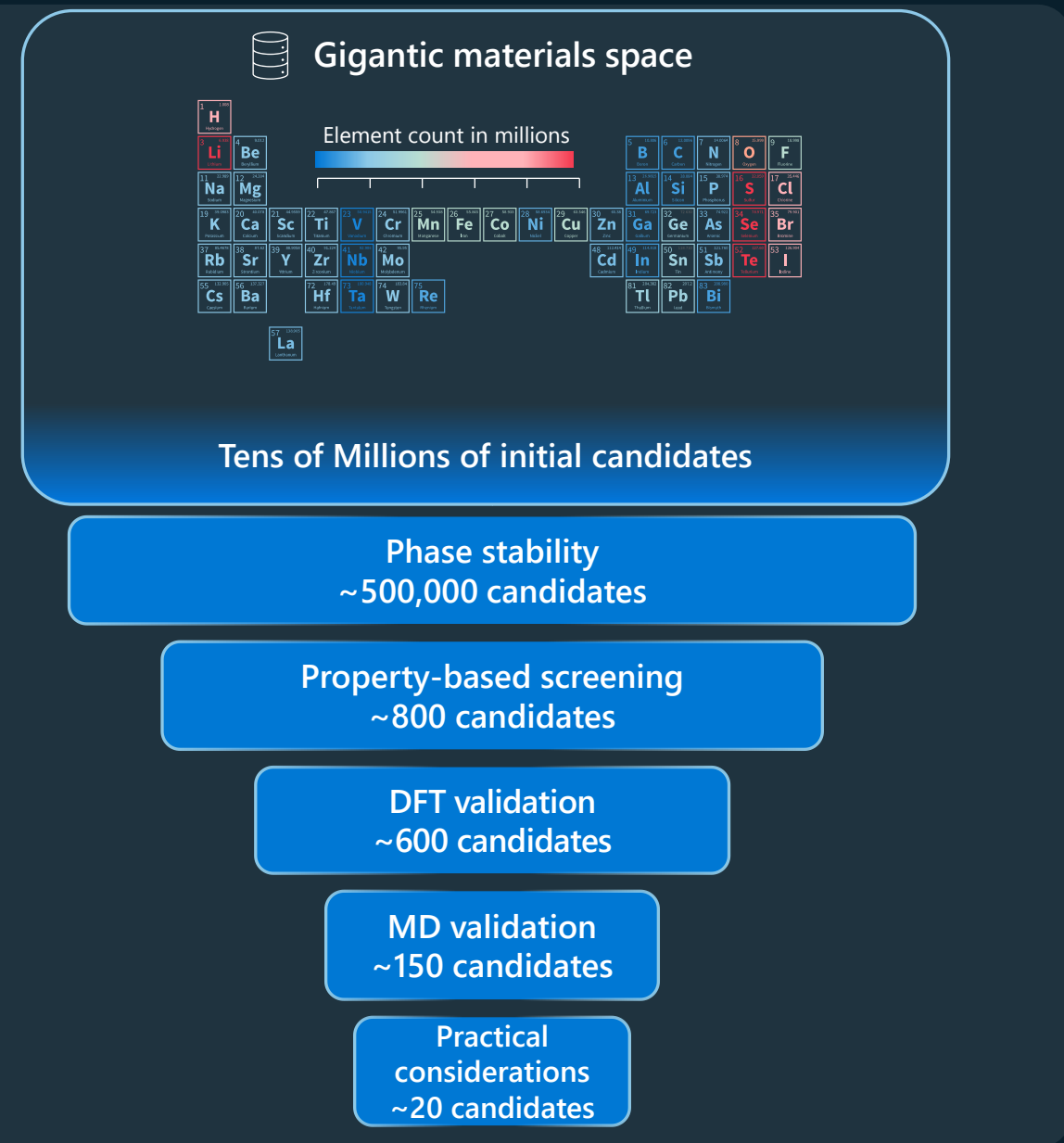


Accelerating chemical and materials discovery with AI Services

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



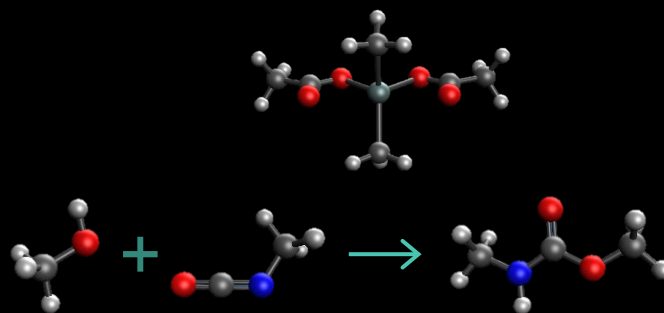
From 1K to 30M initial candidates (30,000x search space)

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).

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](#).