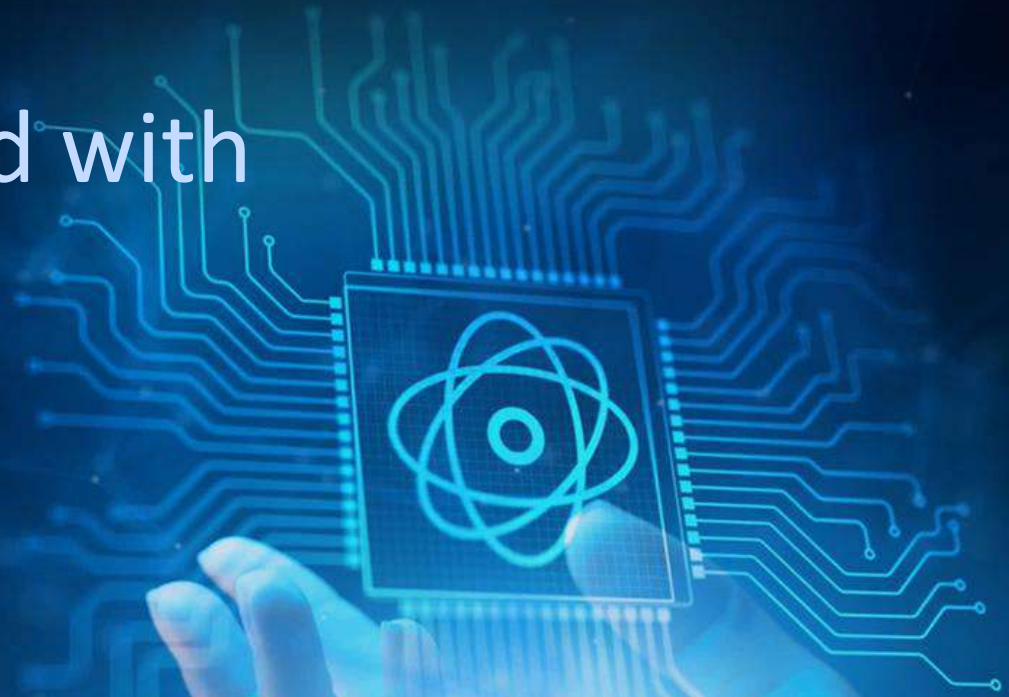
Experience Quantum Advantage with HI-VQE

Chemical Accuracy achieved with Hybrid Quantum-Classical Computational Chemistry



JHPC-Quantum Symposium

J.K. Kevin Rhee

Qunova Computing, Inc.

www.qunovacomputing.com

Quantum Advantage

Criteria that shift users from
classical computing to quantum computing

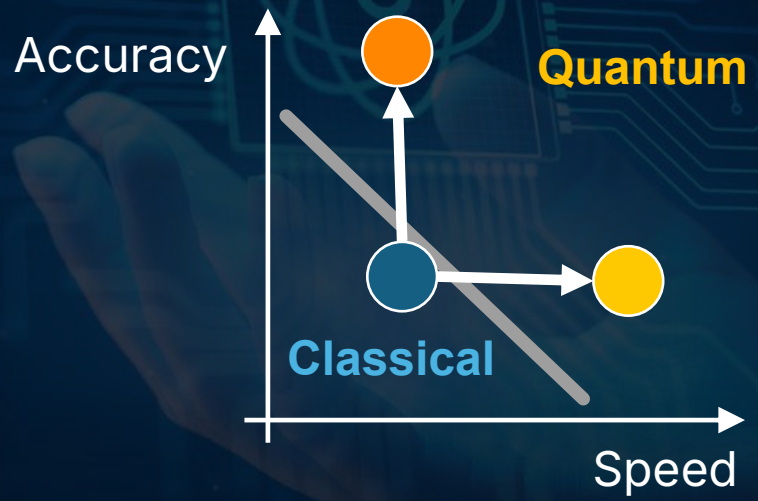
Two types of Technical Criteria

Performance

Accuracy & Capacity

Cost

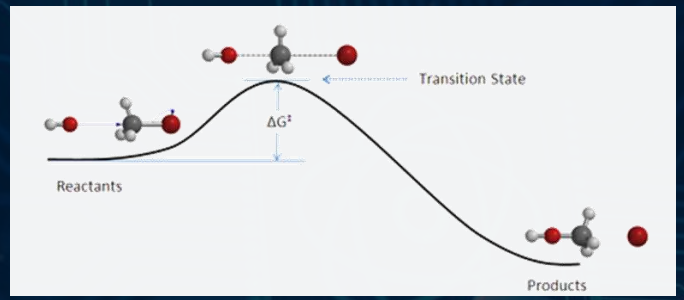
Time & Space

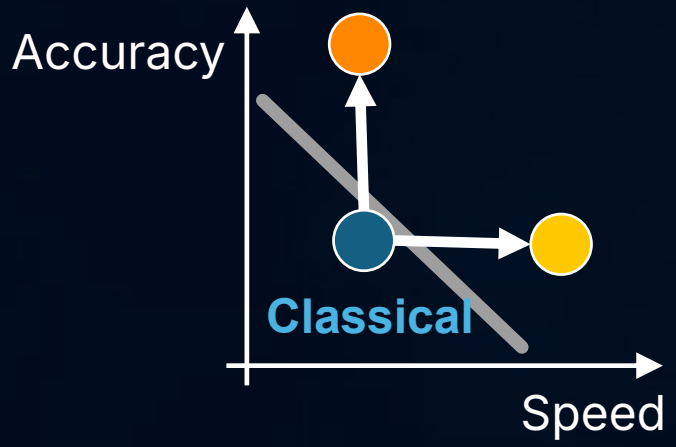


Quantum Advantage in Chemistry

- For the same accuracy, can we compute faster by all means of computing resources ?

Chemical Accuracy ~ 1.6 mHa or 1 kcal/mol





Can quantum computing find more accurate energy for large chemical/physical system?

Eg $\langle H \rangle_{\mathrm{Q}} < \langle H \rangle_{\mathrm{DMRG}}$ or

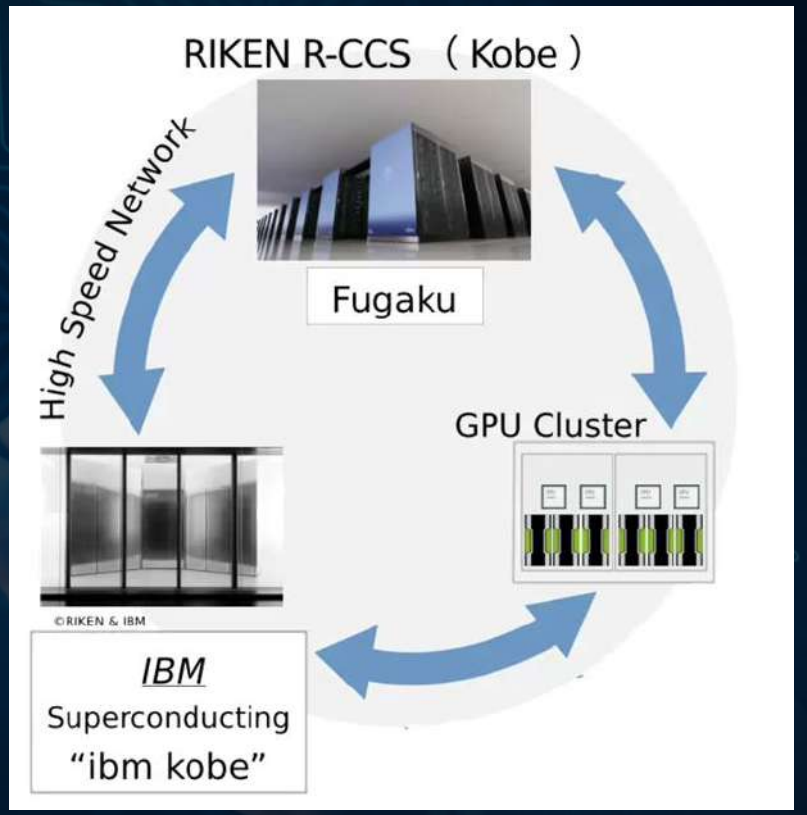
$\langle H \rangle_{\mathrm{Q}} < \langle H \rangle_{\mathrm{HSCI}}$

Can quantum computing find the same accurate energy faster ?

with polynomial or better scalability.

The world best computing resource:

JHPC Quantum: Hybrid Quantum-Classical Platform



Low Cost and Accurate Hybrid algorithm

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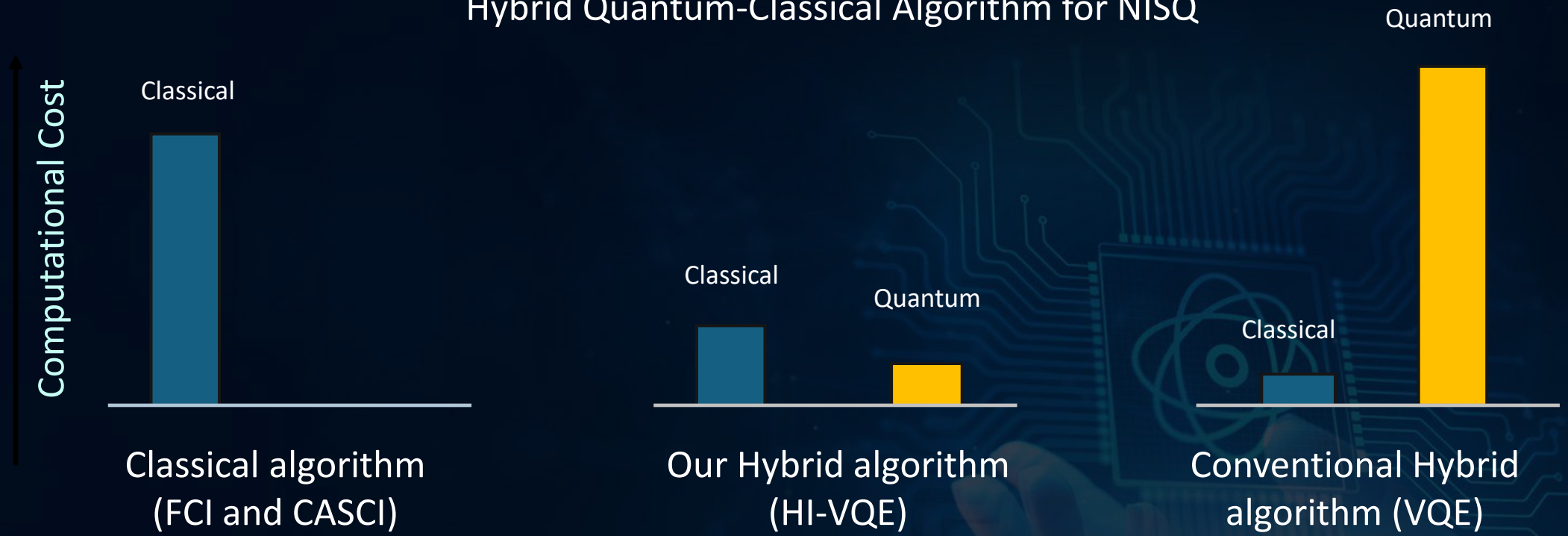
Hybrid Quantum-Classical Algorithm for NISQ



Classical algorithm (FCI and CASCI)

- Purely classical
- Most Accurate without noise effect
- Expensive using CPU

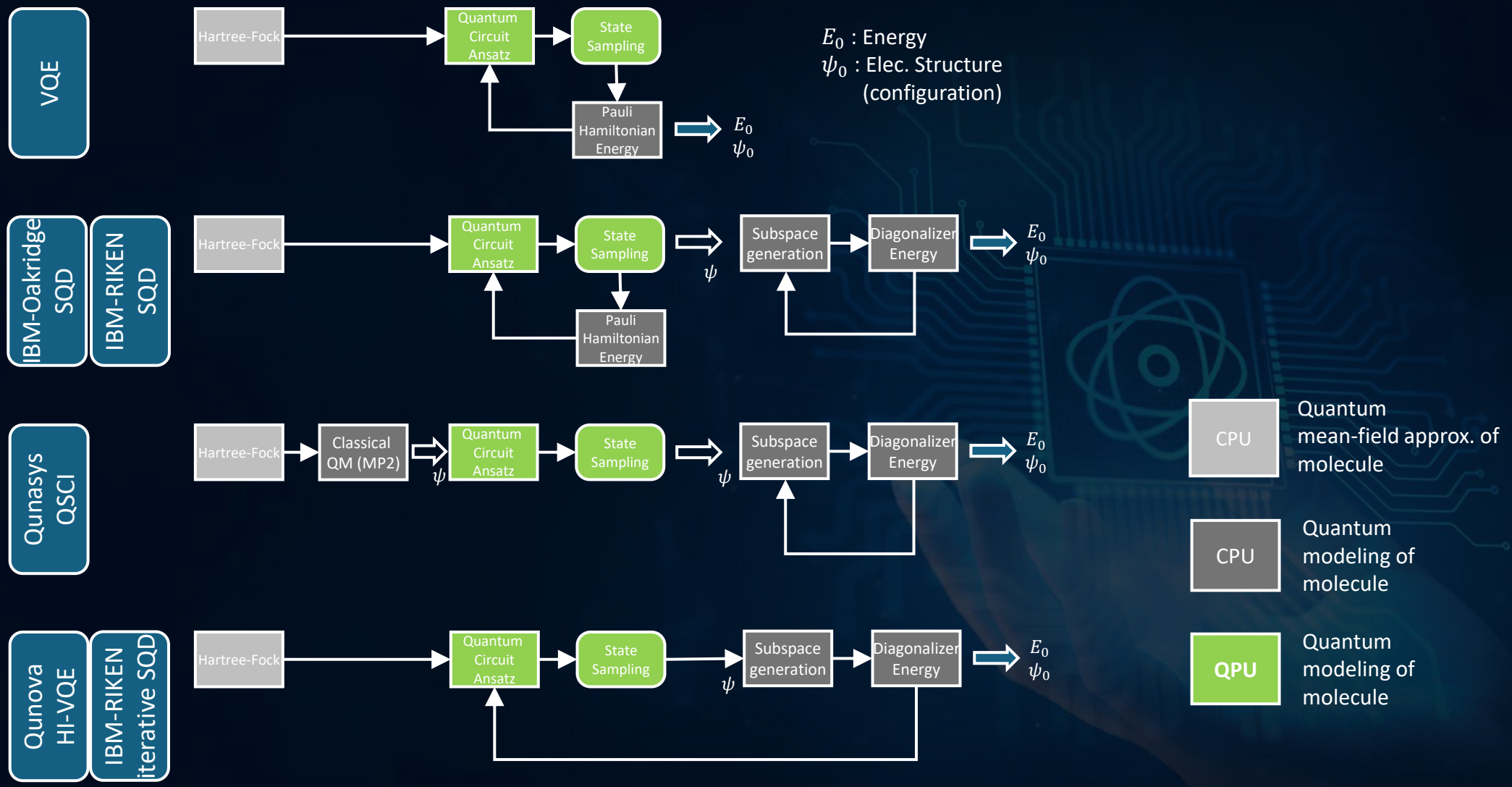
Our Hybrid algorithm (HI-VQE)

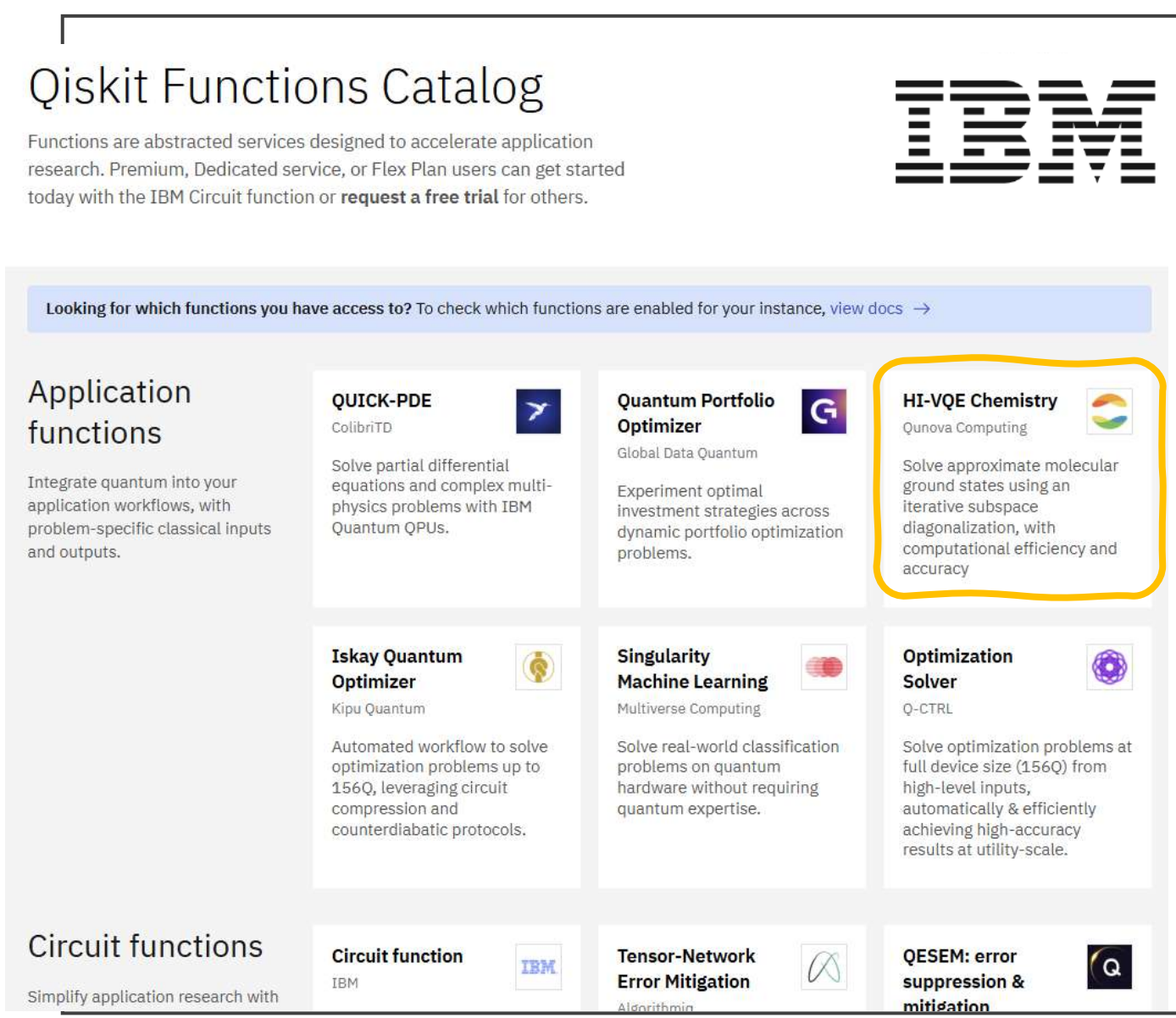
- Minimize the cost
- Accurate with little noise effect
- Useful results up to 60 qubits

Conventional Hybrid algorithm (VQE)

- Expensive with NISQ
- Limited accuracy with Noise
- Useful results up to 20 qubits

Zoo of Hybrid Algorithms for Hamiltonian Simulation





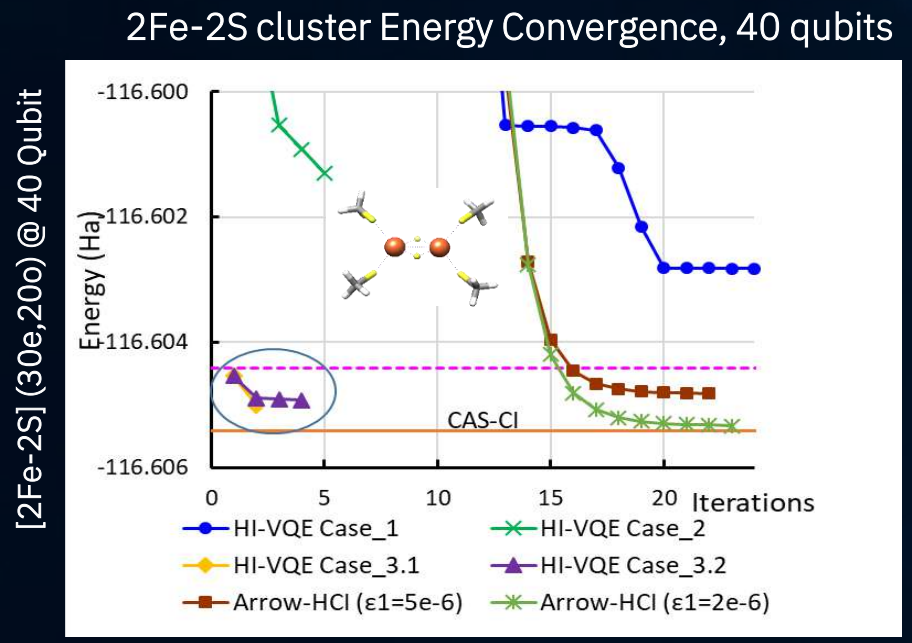
HI-VQE

@ qiskit functions catalog

HI-VQE = Iterative SQD

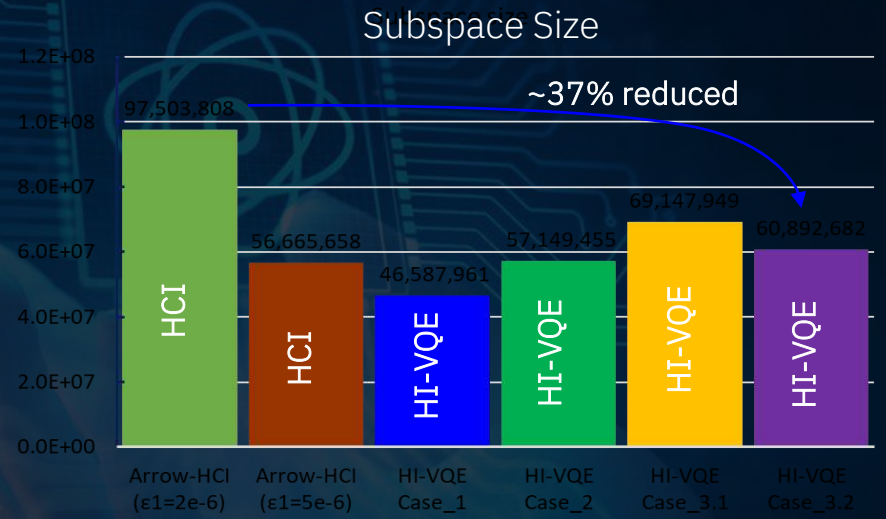
The sole chemical analysis solution in the catalog

Achieving Chemical Accuracy: 2Fe-2S 40 qubits, IBM Fez



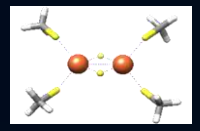
HI-VQE efficiently manages the variational space by intelligently and **iteratively search important states**, and achieves **similar accuracy** with reduced subspaces.

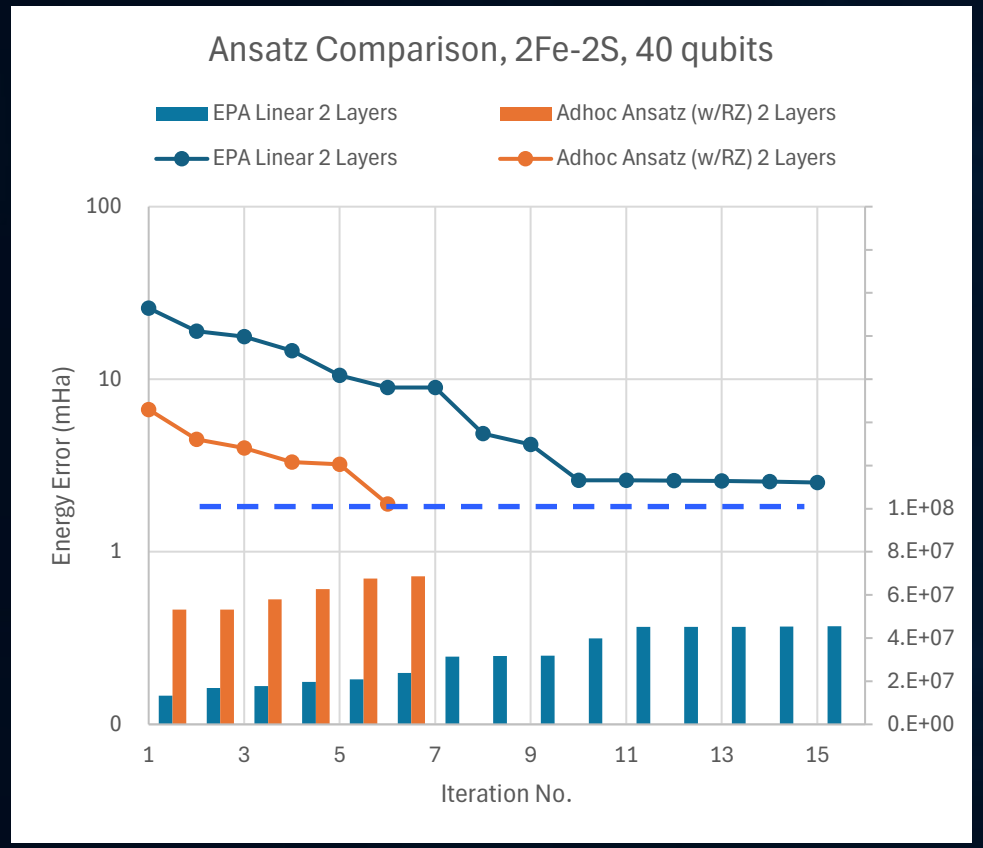
HI-VQE reaches the **chemical accuracy** level with **less iterations** (c.f. HCI).



Achieved similar **accuracy** with **smaller subspace size**

Impact of Ansatz design: 2Fe-2S 40 qubits





- Ansatz 1: EPA 2
  (Excitation Preserving Linear, 2 Layer)
- Ansatz 2: Adhoc 2
  (Interaction Aware Adhoc Givens, 2 Layer)

	EPA, 2 layer	Adhoc, 2 layer
Depth	650	520
2 qubit gate	310	760
1 qubit gate	1700	2930

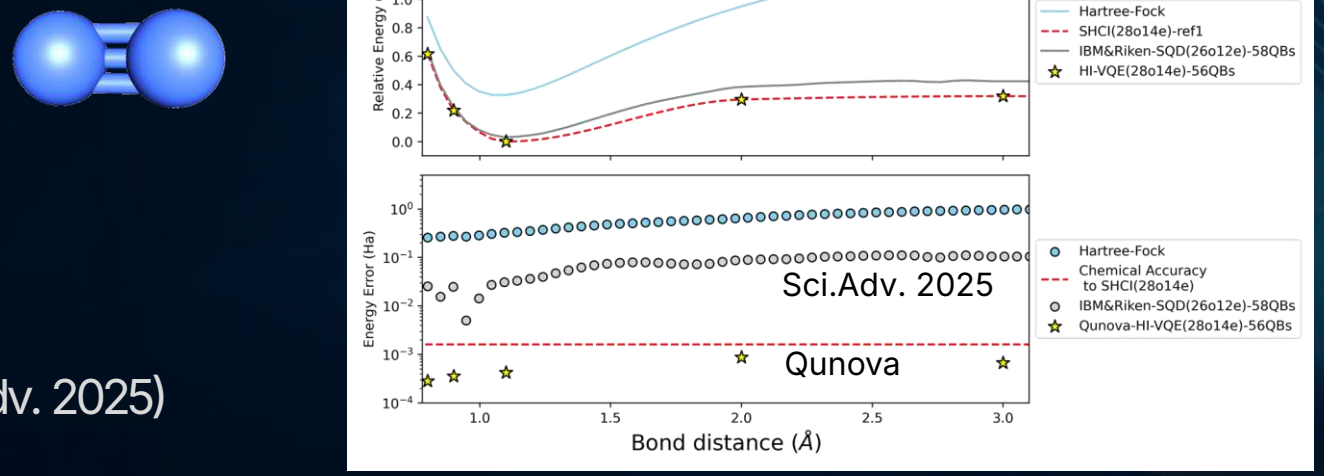
Experience The Quantum Advantage

Within the limit of chemical accuracy,

Qunova Computing's HI-VQE can compute faster in 56 qubit N2 example

with hybrid quantum classical computing using IBM Heron.

HI-VQE for 56-qubit N_2 (28o 14e) PES



* HI-VQE = iterative SQD (Sci.Adv. 2025)

Experience The Quantum Advantage

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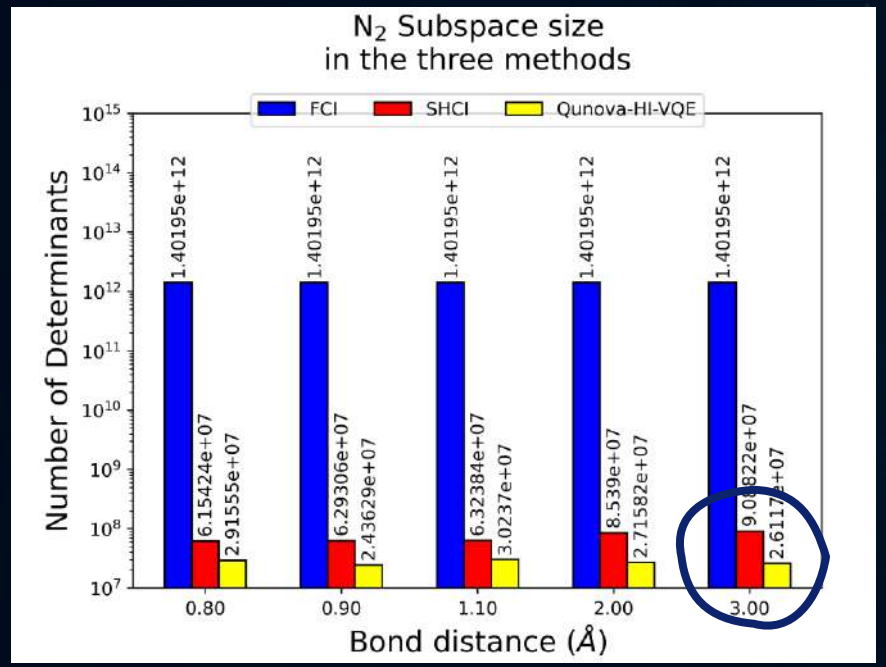
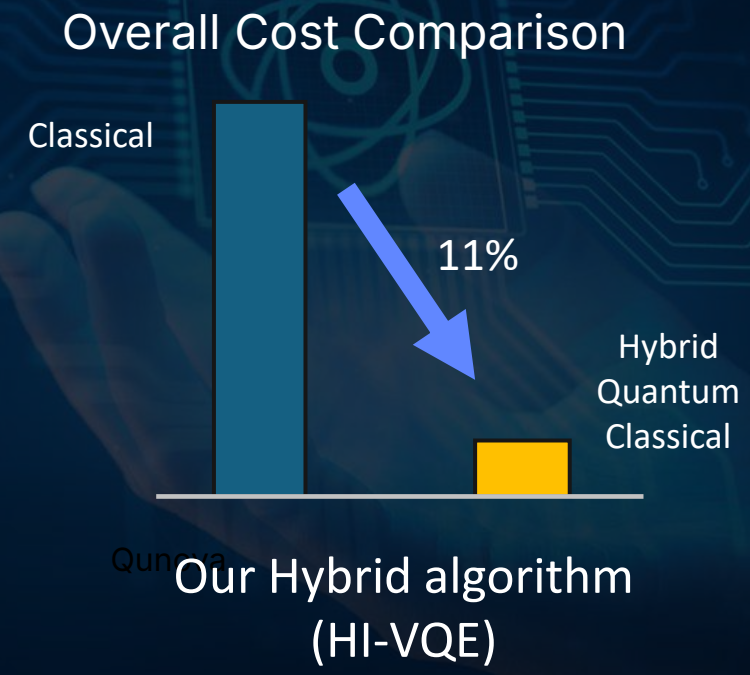
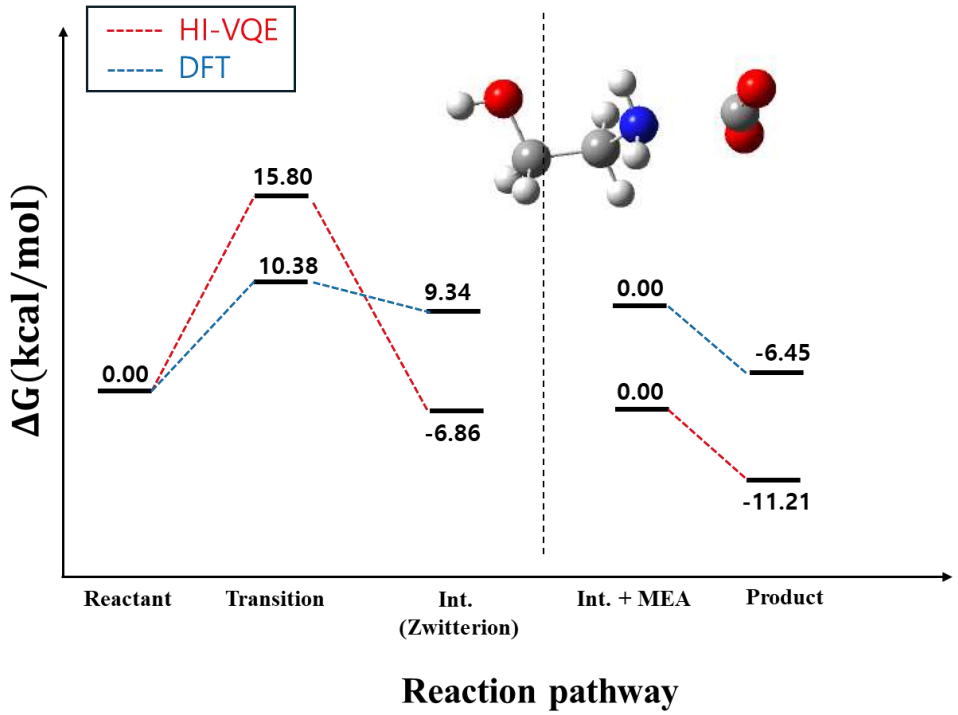


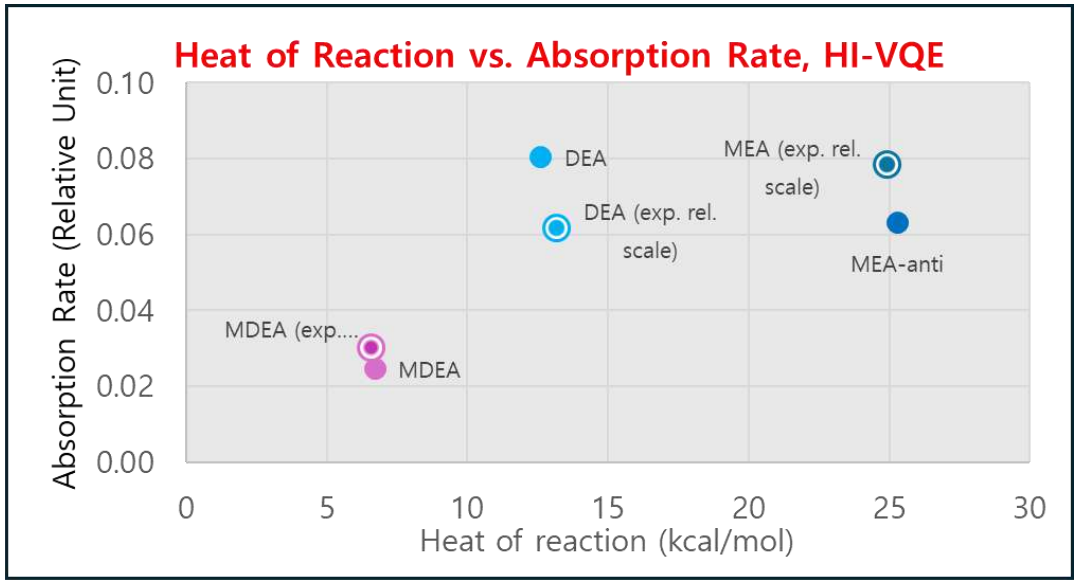


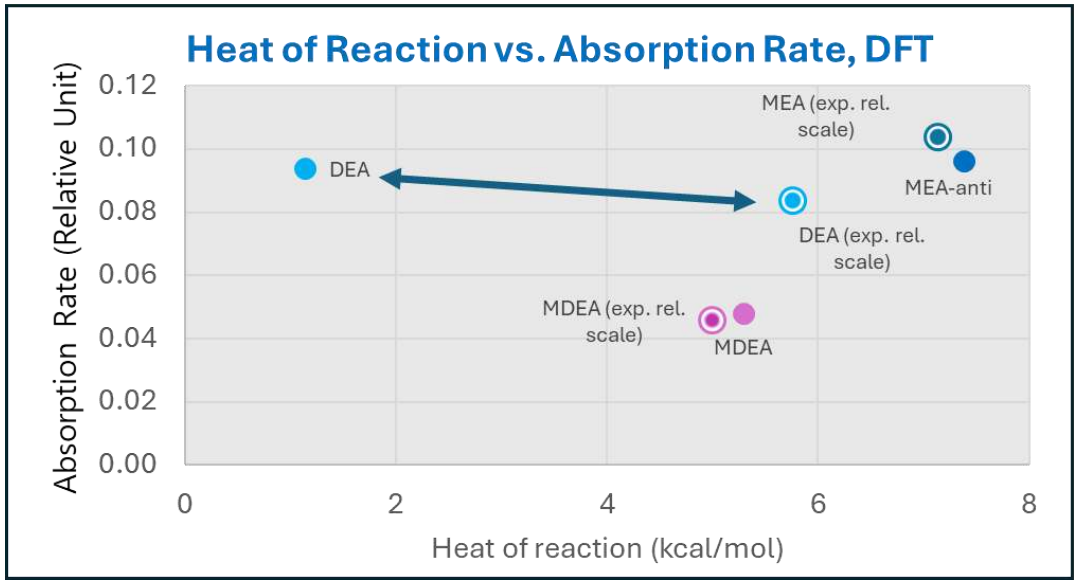
Qunova HI-VQE with implicit solvent effect, 48 qubits – Reaction pathway calculation of carbon capture

- Molecule: MEA(1st amine), DEA(2nd amine), MDEA(3rd amine)
- DFT (classical simulation): Full orbital space
- HI-VQE (Quantum simulation): 24 active orbital(AVAS), 48 qubits
- Activation and reaction energy calculation for amine type carbon capture molecules
- HI-VQE and DFT exhibit different trend in the reaction pathway of MEA
- The analysis of absorption rate and heat of reaction for MEA, DEA, and MDEA shows that **HI-VQE yields trends more consistent with experimental results compared to DFT calculation.**

MEA reaction pathway







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Emerging Quantum Advantage

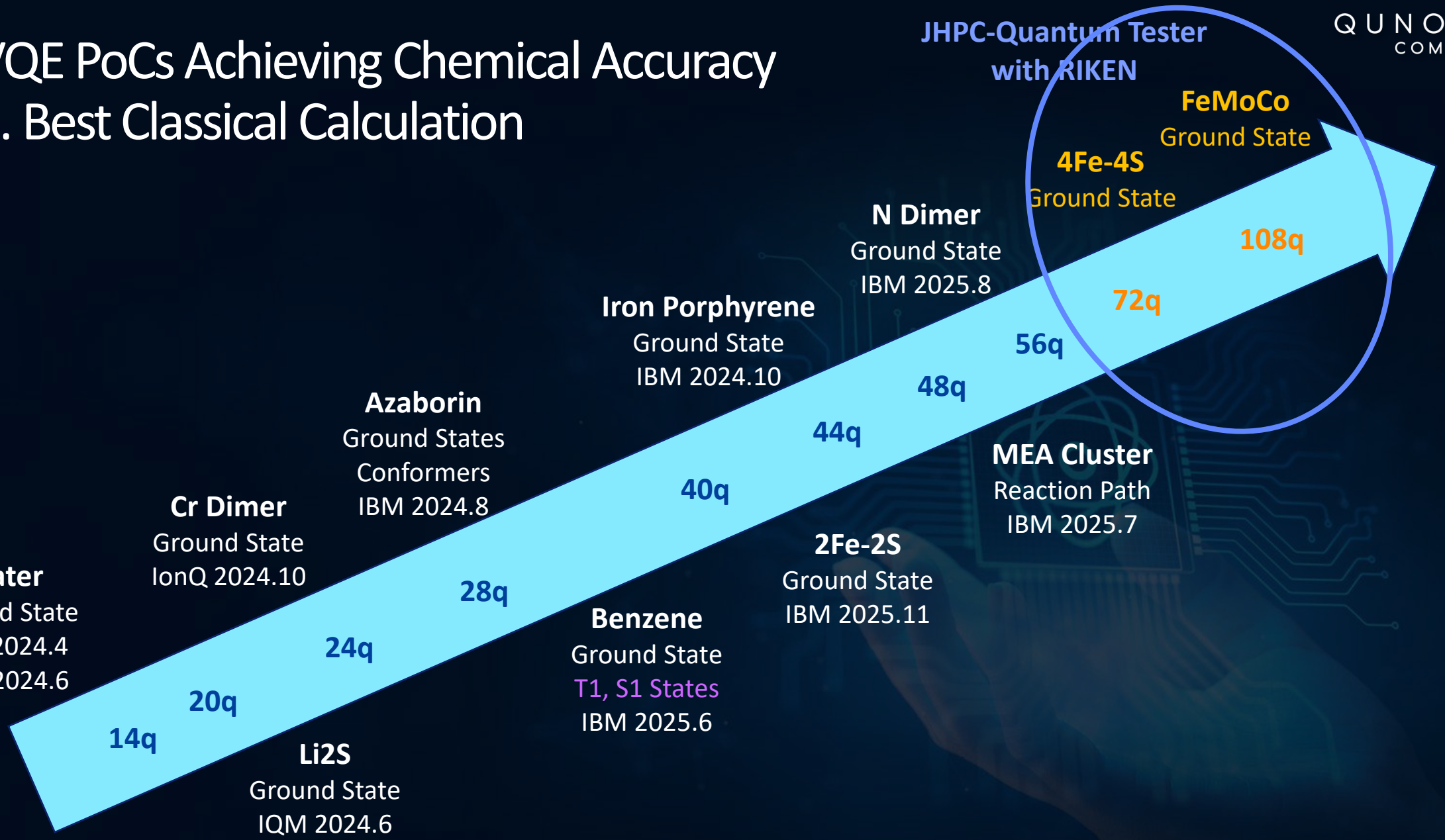
Year	Algorithm / Approach	System / Molecule	Qubit Count	Accuracy (mHartree)	Achievement	Ref
2018	VQE (trapped-ion)	H_2, LiH	4	~1.6	Experimental validation near chemical accuracy	Phys. Rev. X (2018)
2020	Compact VQE	H_2	4	<1.6	Achieved chemical accuracy with compact ansatz	Takeshita et al., 2020
2024	**HI-VQE**	Li_2S, H_2O, CH_4	20–24	1.6	Achieved chemical accuracy on NISQ hardware	Qunova Press arXiv:2503.06292
2025	**HI-VQE**	**N_2**	56	0.2	Large-scale molecular modeling with ultra-high precision	*Qunova Internal Report*
2025	**HI-VQE**	**2Fe-2S cluster**	40	1.0	First chemical accuracy for metal-sulfur cluster	*Qunova Internal Report*
2025	**IBM SQD**	CH_2 (open-shell)	52	~19	Near-chemical accuracy for singlet–triplet gap	IBM Blog Quantum Insider
2025	QPE (Quantinuum)	H_2	56	10^{-10}	Far beyond chemical accuracy	arXiv:2501.xxxxx
2025	IBM+RIKEN Hybrid	Fe–S cluster	77	Goal approached	Large-scale hybrid simulation (explicit chemical accuracy not claimed)	Science Advances

Note:

HI-VQE is equivalent to Iterative SQD

HI-VQE results are obtained on various IBM System 2 HWs.

HI-VQE PoCs Achieving Chemical Accuracy w.r.t. Best Classical Calculation



• Forward Looking Use Cases

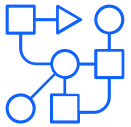
Computational Chemistry

- Requires massive computational power to accelerate R&D pipelines
- **HI-VQE delivers quantum-level accuracy with significant gains in speed and cost**
- Solves highly complex chemistry problems:
- • Ground & excited state energies
- • Reaction pathway analysis
- • Binding affinity calculations

Hybrid quantum–classical computing surpasses top classical limits, opening a new era of quantum chemistry

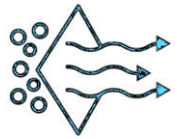
Material Design & Drug Discovery

- Chemical design requires navigating an enormous, complex chemical space
- Current virtual design tools explore up to 10^{20} compounds, yet struggle with accurate de novo design
- Classical approximations limit precision and reliability
- **HI-VQE with fragment-based screening and advanced design platforms, the searchable chemical space expands to 10^{40}**
- **Enables accurate exploration of entirely new molecular designs**



Logistics & Finance

- Logistics and financial operations require solving large-scale, complex optimization problems
- Current NISQ hardware handles only tens of parameters, limiting practical use
- **HI-VQO expands solvable problem sizes to thousands–20,000+ parameters**
- **Enables high-accuracy, efficient decision-making beyond classical limits**
- Unlocks quantum-enhanced optimization for routing, scheduling, portfolio design, and risk analysis



Structural & CFD Design

Advanced mechanics and robotics product design require solving large-scale, complex CFD problems

Current PDE solvers can handle only thousands of grid point modeling, limiting practical use

HI-VQMP expands solvable problem sizes to 1 billion grid point analysis for non-linear CFD PDEs

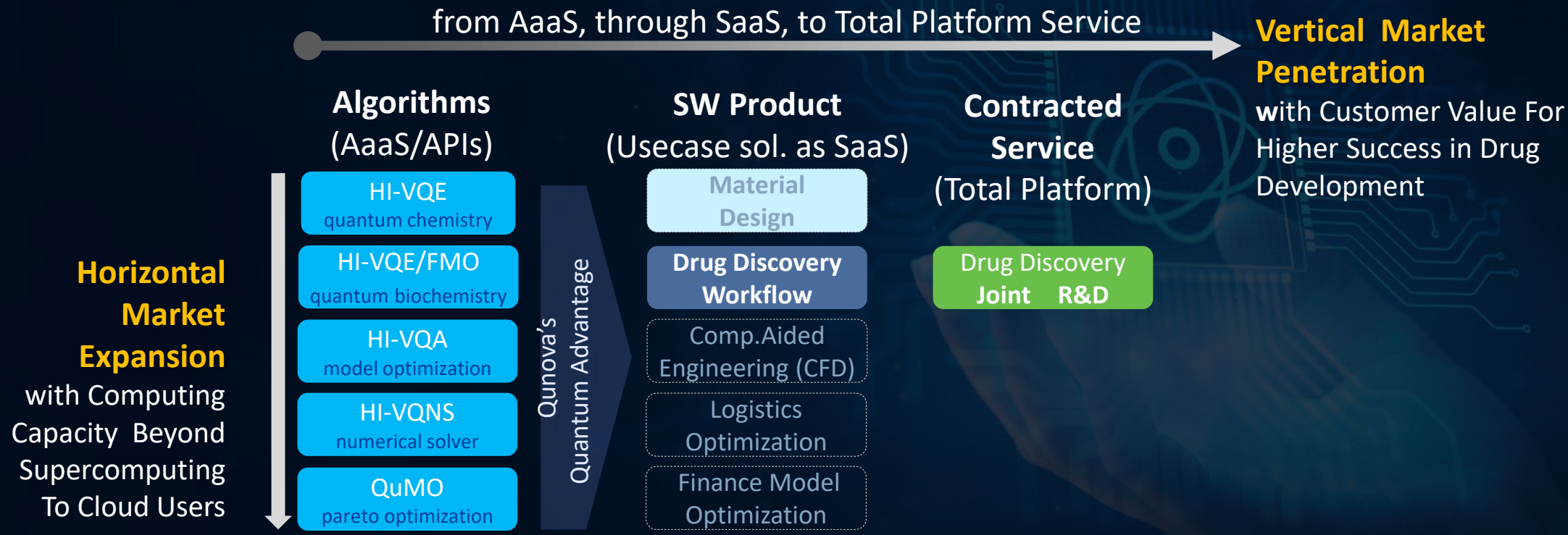
Enables high-accuracy thermo-mechanical engineering beyond classical limits

Unlocks quantum-enhanced mechanical, aerospace, delicate robotics product designs.

Vision, Mission & Strategies

Mission Providing unrivaled Quantum Algorithm solutions to customers in diverse verticals. And expand target verticals with Qunova's best practices.

Vision Providing computing software innovation to customers based on the most advanced **Quantum Advantage**



Thanks for Attention

and Q&A

Contact:

Jay Kim	COO/Qunova	jay.kim@qunovacomputing.com
Kevin Rhee	CEO&CTO/Qunova	rhee.jk@qunovacomputing.com
Taeyong Cho	CEO/Cho&Company	mountain@cho-co.jp