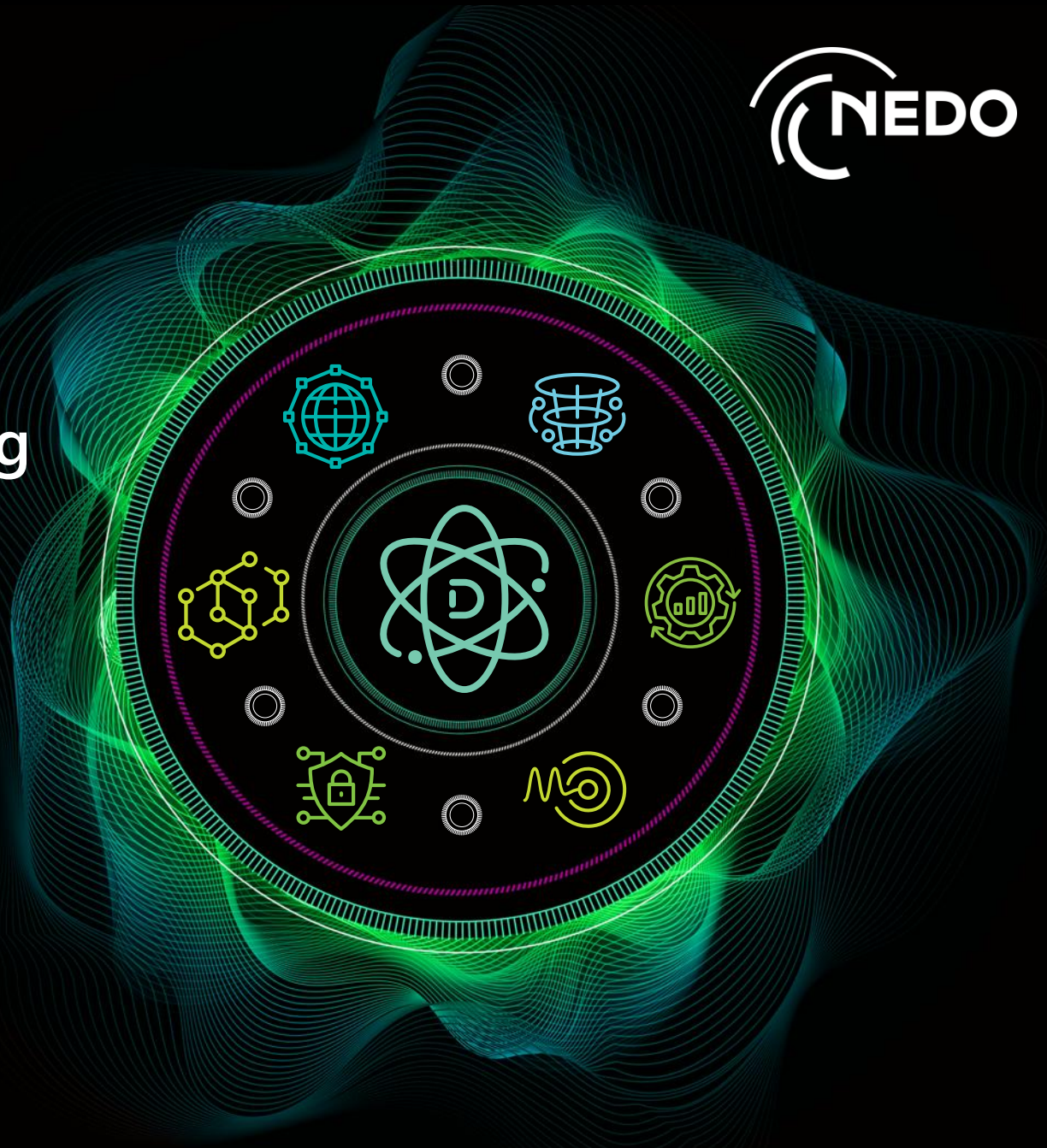
Quantum Computing Use Cases

High-Accuracy Materials Screening Through Integration of Quantum Computers and HPC

SoftBank Corp.



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

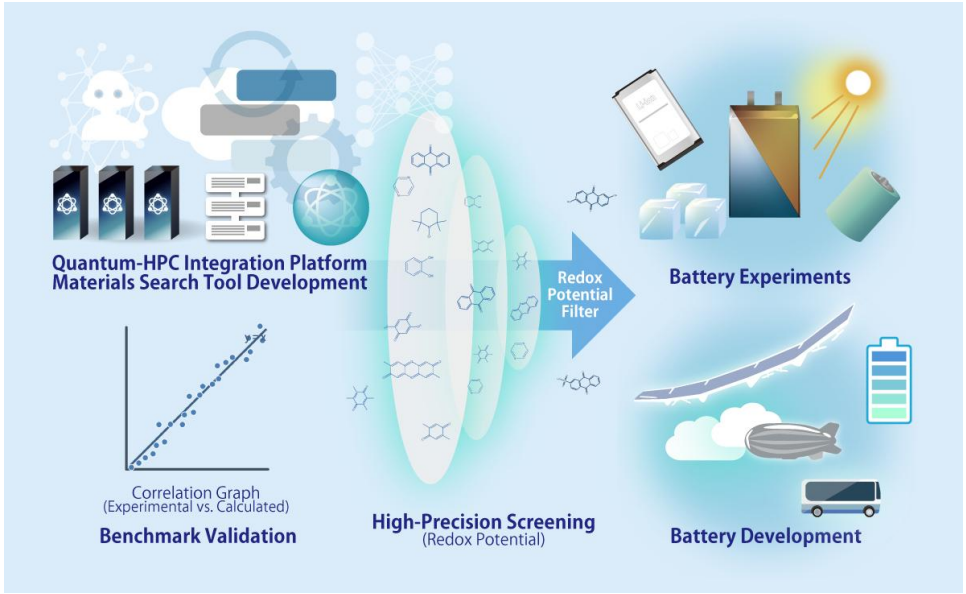
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Process	material search
Method	Simulation
Category	Gate*

Background

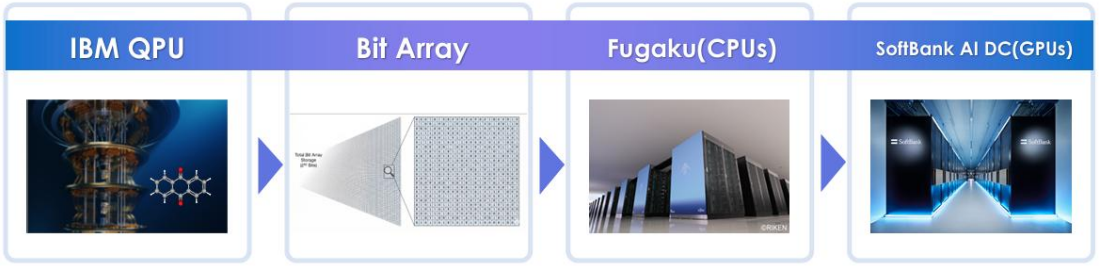
- Next-generation devices such as electric vehicles, drones, robots, and HAPS (unmanned aircraft that provide communication networks from the stratosphere) **require next-generation batteries that are lightweight and can operate for long periods**. To realize this, **materials with high gravimetric energy density are needed, but the number of candidates is enormous, making manual evaluation impractical**
- It is necessary to narrow down candidates through computation, but **the accuracy of conventional methods varies depending on the conditions, and high-precision calculation is difficult even with supercomputers**. Quantum computers are expected to help overcome this limitation, and SoftBank Corp. and the Center for Quantum Information and Quantum Biology (QIQB) at The University of Osaka jointly developed **a quantum-HPC linked method**. In the JHPC-quantum test user program, SoftBank built and executed a workflow using IBM Heron, *Fugaku*, and the SoftBank AI Data Center

Issues and motivation to be solved

- This use case aims to establish a method for accurately predicting redox potential, which is related to gravimetric energy density, and for ranking promising organic molecules before experimentation. **Previous quantum chemistry studies using quantum computers have mainly focused on comparing computational methods for a small number of molecules, and their effectiveness for materials screening based on comparison with experimental values for practical implementation had not been sufficiently evaluated**
- Therefore, 11 organic molecules were examined, and calculated values were systematically compared with experimental values. **Taking into account both overfitting to a single experimental value and uncertainty in the experimental values themselves, the general applicability of candidate ranking was evaluated from the perspectives of both correlation and error**



Conceptual diagram illustrating the framework in which materials screening using a quantum–HPC integrated platform accelerates materials development



Conceptual diagram of the quantum–HPC integrated workflow constructed in this use case

Reference: "Toward Practical Materials Screening Beyond 50 Qubits Enabled by QSCI-AFQMC in a Quantum-HPC Workflow" (https://indico2.riken.jp/event/5118/contributions/28546/attachments/14756/22654/Toshihiro_Aoki.pdf)
Frontier, Journal of the Japan Society of Theoretical Chemistry, April 2026 issue, "Quantum-HPC Integration for Chemical and Materials Simulation: Frontiers and Beyond" (https://www.jstc.org/frontier30/)
*Gate（gate-based）: A computing approach in which operations are applied sequentially to qubits to perform calculations. Similar in concept to logic circuits in classical computers, it can address a wide range of problems.

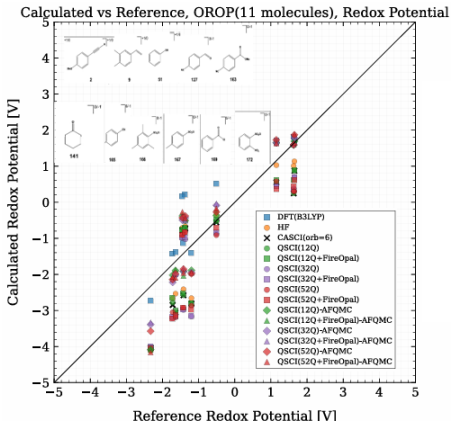
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Problem formulation for quantum computer

- **To calculate 11 organic molecules with accuracy comparable to experimental values, considering all orbitals would require the equivalent of 276 to 528 qubits, which cannot be executed on current QPUs.**
- **Therefore, referring to the division of roles between quantum computers and HPC shown by the SQD method, which has pioneered quantum chemistry calculations beyond 50 qubits and driven quantum-HPC linked research, the QSCI method (a method that uses a QPU to select important electronic configurations) was adopted and extended to support quantum-HPC integration**
- **Important electronic configurations of 12 to 52 qubits are extracted using the QPU and calculated on Fugaku. In addition, electron correlation in orbitals that current QPUs cannot handle is corrected with high accuracy using the SoftBank AI Data Center, and redox potentials comparable with experimental values are obtained**. Under the largest conditions in this use case, the number of electronic configurations to be considered reaches about 10^14. Exact calculation handling all electronic configurations, or exact emulation of the corresponding quantum states, is difficult even on supercomputers, so there is value in using a physical QPU



12Q: (5-7e, 6o), 32Q: (15-17e, 16o), 52Q: (25-27e, 26o)

Method		Correlation coefficient	MAE	MSE
Standard screening baseline DFT(B3LYP)		0.9021	0.5849	0.6276
Quantum-HPC QSCI	32Q	0.8815	1.1196	1.5611
	52Q	0.8679	1.1204	1.5187
Quantum-HPC QSCI-AFQMC	32Q	0.9346	0.5480	0.4016
	52Q	**0.9301**	**0.5731**	**0.4632**

Comparison of redox potential predictions by each method for 11 organic molecules
The figure on the left shows the correlation between experimental and calculated values, and the table on the right presents evaluation metrics for selected methods

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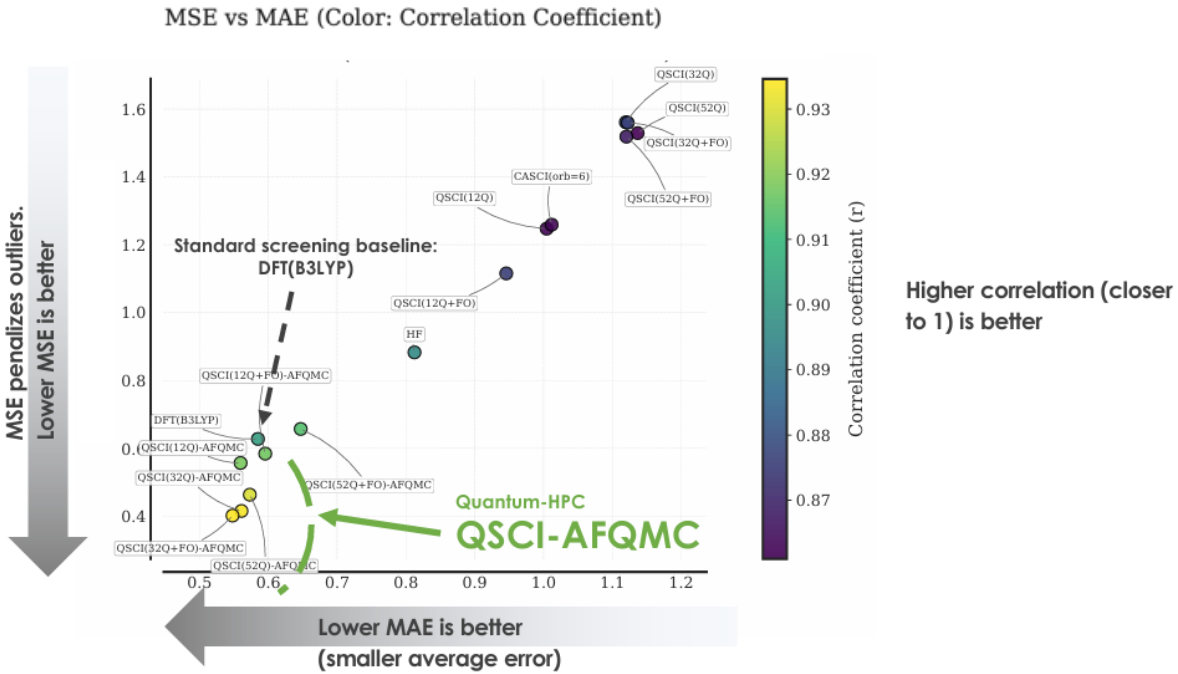
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Expected business benefits

- **This quantum-HPC linked method showed higher correlation with experimental values than the standard method, while maintaining accuracy even in the 52-qubit case**. Through linkage with HPC, it aims to realize practical calculations at an early stage even under the constraints of current QPUs
- **More accurate prescreening can reduce experiments on candidates with low expected performance and reduce rework in candidate selection.** This is expected to shorten research periods and reduce experimental costs, while also accelerating the practical use of promising new materials and compounds.
- In addition, **redox potential prediction may be applicable not only to batteries but also to degradation risk assessment for organic semiconductors and toxicity risk assessment for drug candidates with redox activity, contributing to faster development of new materials and new drugs**



Positioning of each method on the MAE–MSE plane for redox potential prediction
Methods located toward the lower left and shown in brighter colors indicate higher prediction accuracy relative to the experimental values

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More use cases are available on our website. We invite you to explore them.
https://www.quantum-computing-use-cases.nedo.go.jp/english/

More Use Cases

New Energy and Industrial Technology Development Organization (NEDO)
AI and Robotics Department (e-mail: quantum_ai@ml.nedo.go.jp)

This collection of use cases was obtained as a result of the work commissioned by the New Energy and Industrial Technology Development Organization (NEDO) "Cyber-Physical Development Business of Quantum/Classical Hybrid Technology/Study of Use Case of Quantum Technology" and the “Post-5G Information and Communications System Infrastructure Reinforcement R & D Project (Quantum Industrialization)/Comprehensive Study for Promoting the Industrialization of Quantum Computers”.