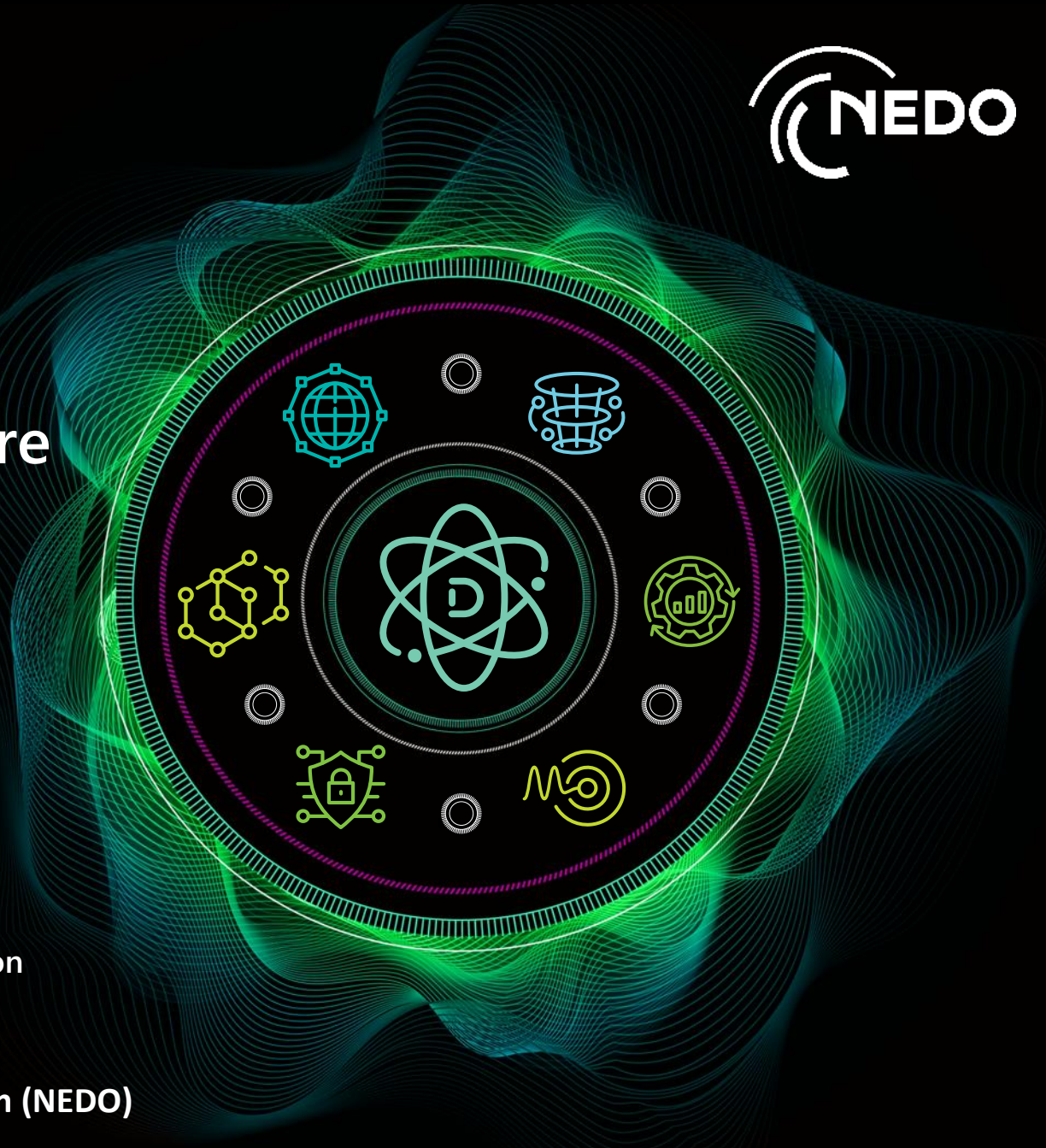
Quantum Computing Use Cases

Organic Molecular Crystal Structure Prediction



Combinatorial Optimization Problem

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New Energy and Industrial Technology Development Organization (NEDO)

【Validated】Organic Molecular Crystal Structure Prediction

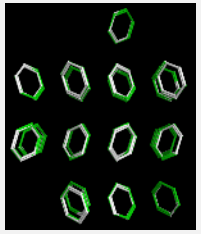
Stable Structure Prediction Workflow

Force Field Development

Stable Crystal Structure Candidate Generation

安定結晶構造候補取得

Stable Crystal Structure Determination



Benzene Crystal Structure

ユースケース概要 Use Case Overview	Prediction of stable crystal structures of organic molecules in drug discovery and materials informatics".
解決できる課題と効果 Issues to be addressed and their effects	Enhancing the stability and ensuring the efficacy of pharmaceuticals and functional materials"
量子技術の貢献 Contributions of quantum technology	Improving the efficiency of the candidate retrieval step in the stable structure prediction workflow for molecular crystals".

実現予想時期 Expected realization period	2025～2030
産業分類 Industry classification	Manufacturing（Materials）
関連するQRAMI階層 Related QRAMI layers	Functional layer
関連する量子技術 Related quantum technologies	Quantum Computer

新規性 Novelty	Minor improvements
達成難易度 Difficulty of achievement	Easy
社会貢献度 Social contribution level	Contributions to a wide range of industries
市場規模 Market size	100B～1T¥

Detail

Organic Molecular Crystal Structure Prediction

Issues to address

- Accelerating and streamlining stable crystal structure prediction of organic molecules for ensuring the stability and efficacy of pharmaceuticals and functional materials

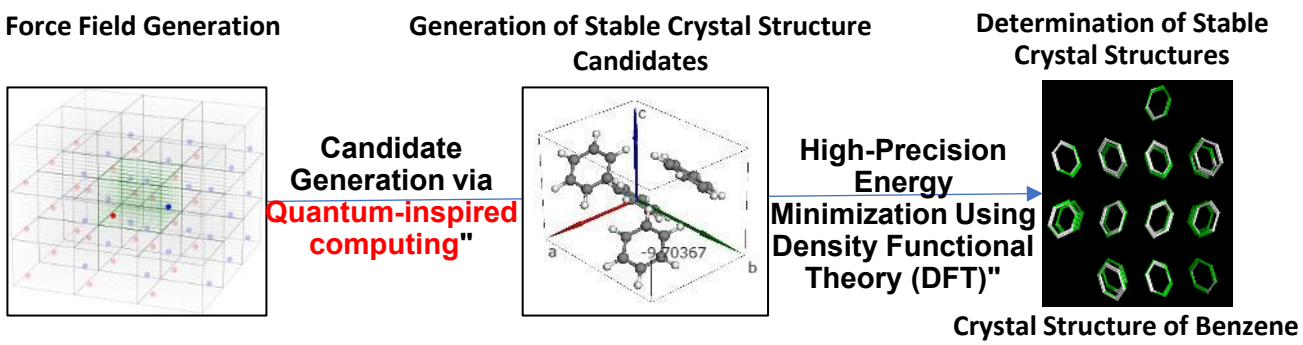
Use case overview

- Enhancing candidate exploring efficiency in molecular crystal stability prediction workflow using quantum technologies (Quantum-inspired technology)"

Implementation vision

Achievement target period: 2030

Stable Structure Prediction Workflow



- Accelerating and optimizing stable crystal structure candidate generation for the design of pharmaceuticals and functional materials

Expected benefits

- Streamlining the design process to ensure the stability and efficacy of pharmaceuticals and functional materials
- Preventing losses due to the emergence of alternative stable crystal forms during manufacturing after drug launch
- realization of novel functional materials

Action plan

QRAMI hierarchy	Action
Business	Establishing applicable technologies for diverse Organic molecules and their use in designing novel functional materials
Function	Accumulation, database development, and utilization of prediction data
Information	Accumulation, database development, and utilization of prediction data
Integration	Quantum-inspired technology, fault-tolerant quantum computing (FTQC), and high-performance computing (HPC)
Asset	Quantum-inspired computing, fault-tolerant quantum computing (FTQC), and high-performance computing (HPC)

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 ”.