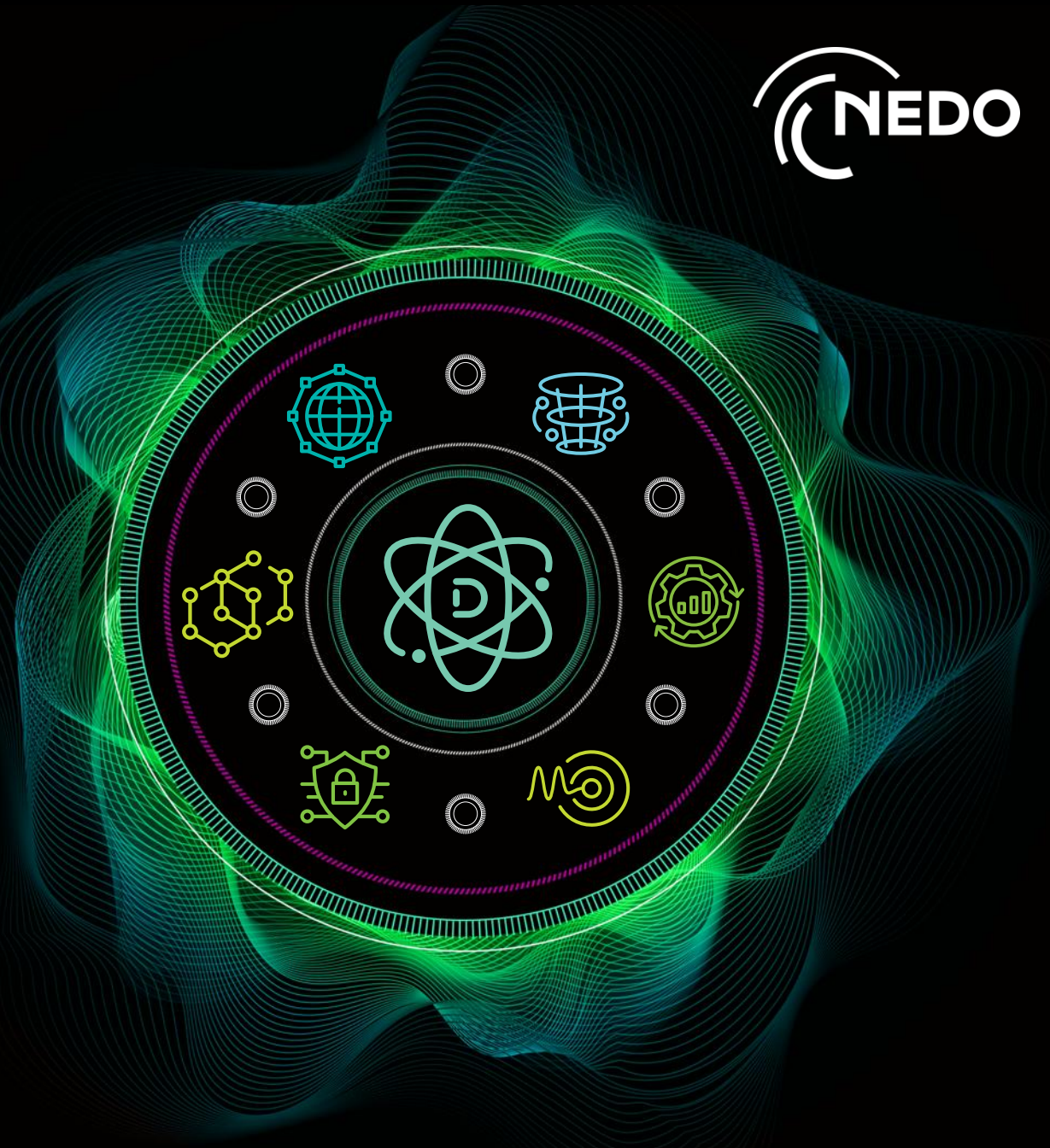
Quantum Computing Use Cases

Modeling of Oxygen Reduction Reaction in Automotive Fuel Cell Development

BMW



New Energy and Industrial Technology Development Organization (NEDO)

BMW: Modeling of Oxygen Reduction Reaction in Automotive Fuel Cell Development [2022/12]

Validation

Industry	Process Manufacturing
Process	research and development
Method	Simulation
Category	Gate*

Background

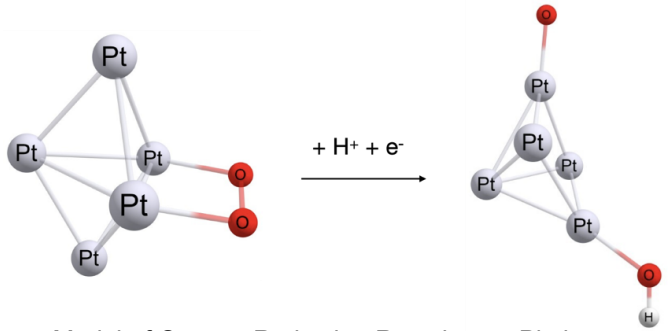
- The slowness of the oxygen reduction reaction (ORR) is an important issue **in the development of new fuel cell technologies for automobiles.**
- Most studies on atomic modeling of catalytic and electrocatalytic chemical reactions, such as ORR, use density functional theory (DFT), which is **limited in computational accuracy.**
- It is known that **DFT calculations fail** for systems in which strong (static) electronic correlations are involved, such as metal complexes (compounds in which metal and non-metal atoms are bonded) and transition states.

Issues and motivation to be solved

- By utilizing quantum computers, it is expected that **complex systems can be accurately calculated using first principles** without losing accuracy using approximate methods such as DFT.
- BMW has **demonstrated the ORR mechanism for the oxygen reduction reaction on platinum clusters.**

Problem setting as a quantum computer

- Targeting the oxygen reduction reaction on a platinum cluster, **using quantum computers to calculate the ground state energy** of the interaction between platinum cluster and oxygen
- This use case **leverages quantum simulations from Amazon Braket, AWS's quantum computing service, using InQuanto, Quantinuum's quantum computing science software platform**.
  - ✓ To perform quantum chemistry calculations, **assume that the gate method (simulation) is used**



Model of Oxygen Reduction Reaction on Platinum Clusters

Expected business benefits

- **We have constructed a minimal model of the reaction steps occurring on platinum clusters and performed an exploratory calculation of their ground state energies.**
- This use case was interesting to BMW because it **could be applied to vehicle fuel cell design in the future**.

Reference: AWS"Exploring computational chemistry using Quantinuum's InQuanto on AWS" (https://aws.amazon.com/jp/blogs/quantum-computing/exploring-computational-chemistry-using-quantinuums-inquanto-on-aws/)
*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.

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)
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