

February 21, 2023 Atmonia ehf. Fujitsu Limited

## Fujitsu and Atmonia succeed in development of new technology that accelerates search for disruptive catalyst for enabling sustainable ammonia production

# Significant reduction of search times through quantum chemical simulation with HPC and AI

### Tokyo, Japan and Reykjavík, Iceland – February 21, 2023

Fujitsu and Atmonia ehf., an Icelandic start-up company developing a novel method for synthesizing sustainable ammonia, today revealed the latest milestone in their joint research into catalysts for sustainable production of ammonia, by successfully developing a high-speed technology for quantum chemical simulations. By combining this technology with an AI technology for scientific discovery developed by Fujitsu, the two companies succeeded in more than halving the search time for a catalyst material that efficiently synthesizes ammonia from water, air, and electricity at ambient temperatures and pressures.

The two companies carried out various quantum chemical calculations using Fujitsu supercomputing resources based on simulation data for ammonia synthesis owned by Atmonia. Vast amounts of data derived from these calculations, including the structure of atomic configurations and the types and ratios of chemical elements that compose catalyst materials, were used to train an AI simulation model that can rapidly identify catalyst candidates. Fujitsu's AI technology for scientific discovery was also used to identify trends in the properties of materials suitable as ammonia synthesis catalysts based on causal relationships among more than 10,000 cantidadates, helping to narrow down catalyst candidate data. The catalyst's discovery search includes e.g. the type and position of the atoms in the catalysts and the free energies of intermediates in the nitrogen reduction reaction.

Going forward, the two companies will use the newly developed technology to select specific ammonia synthesis catalyst candidates and verify their effectiveness, with the ultimate goal of innovating a sustainable production method for ammonia.

The initiative, which marks the first major development in joint research announced in April 2022, will be showcased at Fujitsu ActiveNow: Technology Summit on February 22 in Silicon Valley.

#### About the newly developed technology and results

1. High-speed quantum chemical calculations technology combining HPC and AI simulation models.

By combining the generation of simulation data to speed up quantum chemical calculations with HPC and train AI simulation models to predict unknown data, the two companies have developed technology that significantly increases the efficiency of catalyst search.

Using the relationship between the input and output of the quantum chemical calculations data obtained by HPC as the training data, a new AI simulation model was devised by efficiently performing training specialized in the material search of the target. By inputting structural data, new catalyst material candidates can be predicted 100 times faster than conventional quantum chemical calculations.

2. Properties estimation of compounds suitable for ammonia synthesis by combining highspeed quantum chemical calculations technology and causal discovery technology.

By generating simulation data for more than 10,000 cases of ammonia synthesis catalyst candidates using quantum chemical calculations accelerated by HPC and AI developed, and by applying Fujitsu's unique AI technology for scientific discovery, researchers were able to discover trends in the properties of materials suitable for catalysts based on causal relationships among items in the data such as the type and position of catalyst atoms and the free energies of intermediates. As an example, elements of lower group numbers in the periodic table are more suitable as the base metals in the catalysts. Referring to these trends, the researchers could efficiently determine the direction of material candidate selection.

As a result, the technology allows researchers to automatically narrow down the search range of catalyst material candidates. By streamlining this time-consuming and labor intensive practice using the AI technology for scientific discovery, the two companies succeeded in reducing the search time for catalyst candidates by more than half.



#### **Future plans**

The two companies aim to contribute to carbon neutrality by selecting specific ammonia synthesis catalyst candidates and verifying their effectiveness, making sustainable ammonia synthesis a practical reality.

Fujitsu will also work to further improve the efficiency of materials research with technology developed in collaboration with the University of Toronto that uses Fujitsu's Quantum-Inspired Digital Annealer technology to discover the optimal combination of material element configurations suitable for catalysts. The "<u>Fujitsu Computing as a Service (CaaS)</u>" portfolio is an important <u>Hybrid IT</u> offering under <u>Fujitsu Uvance</u>, delivering users, including customers in the materials sciences, a versatile suite of cloud services that promises to lower the barrier of entry to advanced computing and software technologies. Fujitsu aims to incorporate this technology into its CaaS portfolio in the future.

#### **Related Links**

- Fujitsu and Atmonia leverage HPC and AI technology in joint project to contribute to carbon neutrality (press release, April 13, 2022)
- Joint research paper by Fujitsu and the University of Toronto (December 13, 2022) Accelerated chemical space search using a quantum-inspired cluster expansion approach

#### About Fujitsu

Fujitsu's purpose is to make the world more sustainable by building trust in society through innovation. As the digital transformation partner of choice for customers in over 100 countries, our 124,000 employees work to resolve some of the greatest challenges facing humanity. Our range of services and soulutions draw on five key technologies: Computing, Network, AI, Data & Security, and Converging Technologies, which we bring together to deliver sustainablity transformation. Fujitsu Limited (TSE:6702) reported consolidated revenues of 3.6 trillion yen (US\$32 billion) for the fiscal year ended March 31, 2022 and remains the top digital services company in Japan by market share.

For more information, please see <u>www.fujitsu.com</u>

#### About Atmonia

Atmonia is an Icelandic tech startup company developing a sustainable process for ammonia production. Atmonia's mission is to significantly reduce greenhouse gas emissions with new technologies in the field of ammonia and nitrate production. The company's technology is both economical and environmentally friendly, and will contribute significantly in the fight against global warming. Atmonia's new technology will produce ammonia from air and water and will emit no greenhouse gases, but the current ammonia production method is responsible for 1-2% of the world's anthropogenic carbon dioxide emissions.

For more information, please see www.atmonia.com

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