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

Using AI for sustainable ammonia production

Fujitsu and Atmonia, an Icelandic start-up company developing a novel method for synthesising sustainable ammonia, have 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 synthesises ammonia from water, air and electricity at ambient temperatures and pressures. Ammonia and amines are commonly used in water-based inks and coatings, as well as adhesives. They serve to "dissolve" the acidic resins and stabilise emulsions and pigment dispersions by charge repulsion.

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 candidates, helping to narrow down catalyst candidate data. The catalyst's discovery search includes, for example, 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.

■ NEWLY DEVELOPED TECHNOLOGY

High-speed quantum chemical calculations technology combines 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 specialised 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.

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 labour 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, which uses Fujitsu's Quantum-Inspired Digital Annealer technology to discover the optimal combination of material element configurations suitable for catalysts. The "Fujitsu Computing as a Service (CaaS)" portfolio is an important Hybrid IT offering under Fujitsu Uvance, 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. **PPCJ**

"By streamlining this time-consuming and labour 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."