PFCC Launches Matlantis Atomistic Simulator as Cloud-Based Service

New high-speed, versatile atomistic simulator quickens
discovery and development of new materials

TOKYO – July 6, 2021 – Preferred Networks, Inc. (PFN), ENEOS Corporation (ENEOS) and their joint venture Preferred Computational Chemistry (PFCC) announced today that PFCC has launched Matlantis™, a cloud-based atomistic simulator that significantly accelerates discovery and development of new materials.

PFCC's Matlantis supports large-scale materials discovery by quickly simulating the atomic-scale behavior of various materials. PFN and ENEOS have incorporated a deep learning model into a conventional physical simulator to increase the simulation speed by tens of thousands of times and to support a wide variety of materials. The deep learning model for Matlantis has been trained with a vast amount of atomic structure data generated by physical simulation on PFN's supercomputers.

Key Features of Matlantis
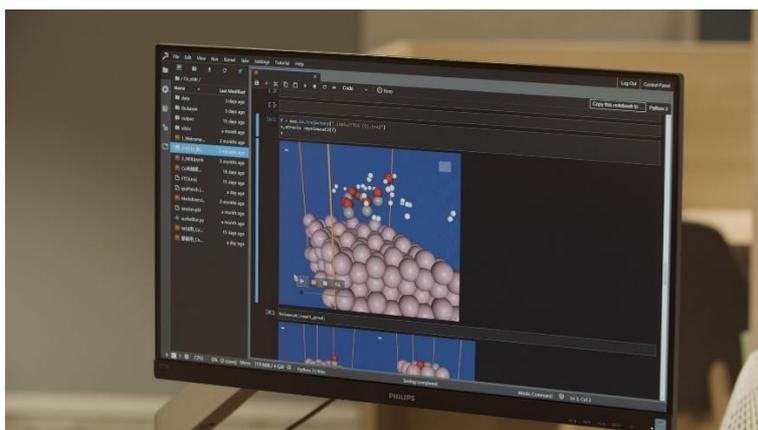
1. **Versatility**
   Matlantis can simulate properties of molecules and crystal systems, including unknown materials. Any combinations of 55 elements are currently supported, and more elements will be added.

2. **High- speed performance**
   The atomistic simulation tasks that take hours to months using conventional DFT (density functional theory) methods on a high-performance computer can be finished in only a few seconds using Matlantis.

3. **User-friendliness**
   Thanks to the pre-trained deep learning model, physical property calculation library and high-performance computing environment, no hardware or software installations are required for performing simulations.

Material simulation on Matlantis screen

The product name Matlantis is a combination of "material" and "Atlantis," a mythical continent appearing in Plato's works that inspired adventurers worldwide. Out of 10^{60} theoretically possible functional molecules, mankind has discovered only a handful of useful materials. The name represents PFCC's commitment to help companies discover innovative materials in the vast ocean of unknown molecules.

Headed by PFN's Chief Operating Officer Daisuke Okanohara, PFCC was established on June 1, 2021 in Tokyo with a paid-in capital of 310 million yen with 51% ownership by PFN and 49% ownership by ENEOS.

"PFCC's mission is to contribute to a sustainable future by enabling companies to create innovative materials," said Daisuke Okanohara, Chief Executive Officer of PFCC. "To achieve this, we have combined Preferred Networks' artificial intelligence expertise and computing infrastructure with ENEOS's expertise in chemistry to build Matlantis. We look forward to providing powerful tools to help researchers worldwide discover game-changing materials that give a positive impact on our future."

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About Preferred Networks
Preferred Networks (PFN) was established in March 2014 with the goal to develop practical, real-world applications of deep learning, robotics and other latest technologies. PFN is currently focused on three priority areas – transportation systems, manufacturing and bio-healthcare – and also exploring the use of deep learning in personal robots, plant optimization, materials discovery, sports analytics and entertainment. In 2015, PFN developed Chainer™, the open-source deep learning framework. PFN's MN-3 supercomputer, which is equipped with the MN-Core™ processor dedicated for deep learning, topped the Green500 list in June 2020 and June 2021. https://www.preferred.jp/en/

About the ENEOS Group and ENEOS Corporation
Under ENEOS Holdings, Inc., the ENEOS Group has developed businesses in the energy and nonferrous metals segments, from upstream to downstream. The Group's envisioned goals for 2040 are: becoming one of the most prominent and internationally-competitive energy and materials company groups in Asia, creating value by transforming our current business structure, and contributing to the development of a low-carbon, recycling-oriented society with the pursuit of carbon neutral status in our own CO2 emissions. ENEOS Corporation, one of the principal operating companies in the Group, is contributing to achievement of the Group's envisioned goals through a broad range of energy businesses.

Matlantis™, Chainer™ and MN-Core™ are the trademarks or the registered trademarks of Preferred Networks, Inc. in Japan and elsewhere.

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