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TerraSky Co., Ltd.

Quemix Launches New Version of Cloud-Based Materials Calculation Platform “Quloud”

Incorporating New Molecular Dynamics Simulation Technology Developed through Joint Research with Idemitsu Kosan

TerraSky Co., Ltd. (Headquarters: Chuo-ku, Tokyo; Representative Director, CEO and President: Hideya Sato) announces that its group company, Quemix Inc. (Headquarters: Chuo-ku, Tokyo; Representative Director: Yuichiro Matsushita; hereinafter “Quemix”), a company engaged in the research and development of quantum computer algorithms and software, has developed, through joint research with Idemitsu Kosan Co.,Ltd. (Head Office: Chiyoda-ku, Tokyo; Representative Director and President: Noriaki Sakai; hereinafter “Idemitsu Kosan”), a molecular dynamics simulation technology that contributes to more efficient materials development, including battery materials. Quemix began offering a new version of its cloud-based materials calculation platform, “Quloud,” incorporating this technology on September 16, 2026.

Background to the Development of the New Molecular Dynamics Simulation Technology and Previous Challenges

In the development of next-generation batteries, molecular dynamics simulations can significantly contribute to reducing prototyping costs and shortening development periods. Practical materials simulations require both interatomic forces and forces exerted by electric fields to be evaluated rapidly and accurately. However, currently prevalent methods face limitations in either computational accuracy or computational speed, which has hindered improvements in the efficiency of materials development.

Characteristics and Technical Limitations of Existing Technologies

Existing technology	Advantages	Disadvantages	Challenges for material systems under electric fields
Kohn–Sham density functional theory (KSDFT)	Extremely high computational accuracy	Computational cost increases in proportion to the cube of the number of atoms	Molecular dynamics calculations for models containing several thousand atoms are virtually impossible
General-purpose machine-learning potentials	Enable fast, large-scale, high-accuracy calculations	Generally do not contain atomic charge information	Difficult to evaluate forces exerted by electric fields, limiting their application to battery materials
Orbital-free density functional theory (OFDFT)	Computational cost scales approximately linearly with the number of atoms, enabling fast charge evaluation for large-scale systems	Interatomic force accuracy is inferior to that of machine-learning potentials	Accurate evaluation of interatomic forces is difficult, making it difficult to ensure the structural stability of materials

Overview of the Jointly Developed New Technology

Quemix and Idemitsu Kosan have successfully co-developed innovative software that combines fast charge evaluation based on OFDFT with highly accurate interatomic force evaluation using general-purpose machine-learning potentials.

This enables molecular dynamics simulations of electric-field-driven ionic conduction in ionic crystal systems and their interfaces while tracking changes in charge over time.

Expected Impact and Future Development

The establishment of this technology makes it possible to directly and dynamically simulate ion motion and charge changes in solid electrolytes and at electrode interfaces under electric fields. This will dramatically accelerate the development of various ionic materials, including lithium-ion battery materials.

Quemix will implement the simulation technology jointly developed through this project as a new feature of its cloud-based materials calculation platform, “Quloud.” Through Quloud, Quemix will provide strong support to companies and research institutions pursuing cutting-edge materials development and contribute to accelerating the development of new materials.

About Quloud, the Cloud-based Materials Calculation Platform

Quloud is a cloud-based materials calculation platform that enables users to perform advanced materials simulations through a web browser. It features an intuitive user interface that seamlessly supports computational methods such as first-principles calculations and molecular dynamics simulations, making it accessible to a wide range of users, from experts to beginners.

Going forward, Quemix will integrate its proprietary quantum algorithms and computational solvers into Quloud. By harnessing quantum computers as computational resources, Quloud will evolve into a next-generation materials development platform that provides powerful support for materials development across the manufacturing industry.

For more information about Quloud:
https://www.quemix.com/en/quloud

Click here for Quemix's press release on this matter:
https://www.quemix.com/en/post/en-20260917-quloud

About Quemix Inc.

Quemix Inc., a consolidated subsidiary of TerraSky Co., Ltd. (Head Office: Chuo-ku, Tokyo; Representative Director Executive President and CEO: Hideya Sato) conducts research and development in quantum computing, quantum sensing, and computational materials science. Under the vision of "realizing the future humanity has dreamed of through quantum technology," Quemix supports breakthrough innovations for companies leading the next generation of quantum technologies.

Since its establishment in 2019, the company has focused on research and development of algorithms for fault-tolerant quantum computers (FTQC), including the development and patenting of the "Probabilistic Imaginary-Time Evolution (PITE®)," a quantum chemistry calculation algorithm with mathematically proven quantum acceleration. As a leading company in FTQC algorithm research in Japan, Quemix is actively advancing research and development aimed at the practical application of quantum computing in materials computation and simulation by 2030.

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