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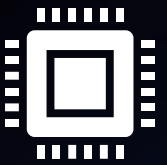
Batteries



Semiconductor packages

HPC & AI: Accelerating materials development

Innovation in Material Design

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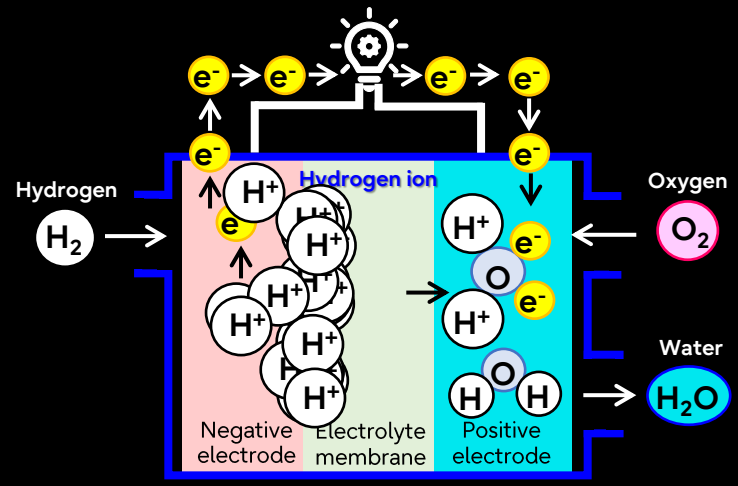
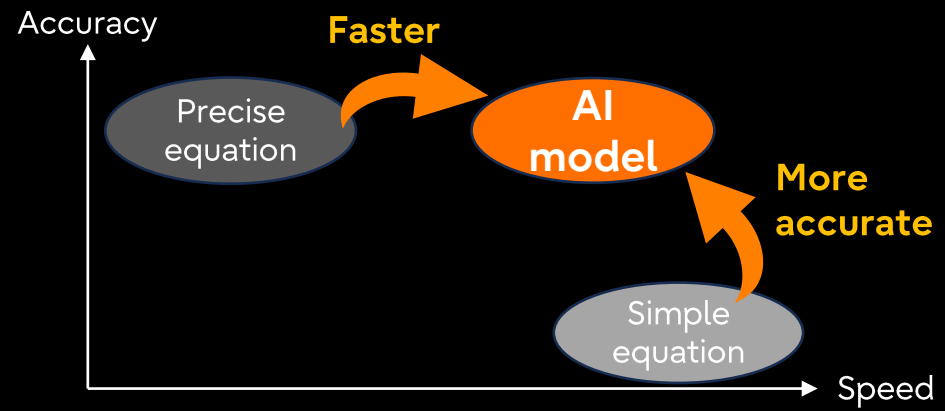
Ex.) Fuel cell

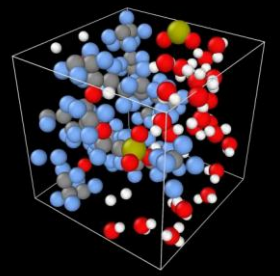


“Hydrogen ions hopping” (Chemical reaction)
is crucial for its performance.

Molecular Dynamics Simulation:
Simulation of atomic behavior to evaluate chemical reactions

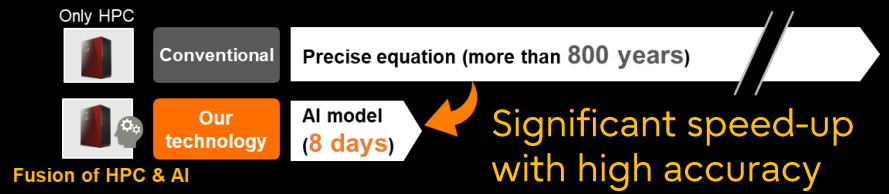


Example of MD simulation



Achieved simulations of > 10,000 atoms and > 10 nano seconds necessary for breakthroughs in material development.

Features of our technology



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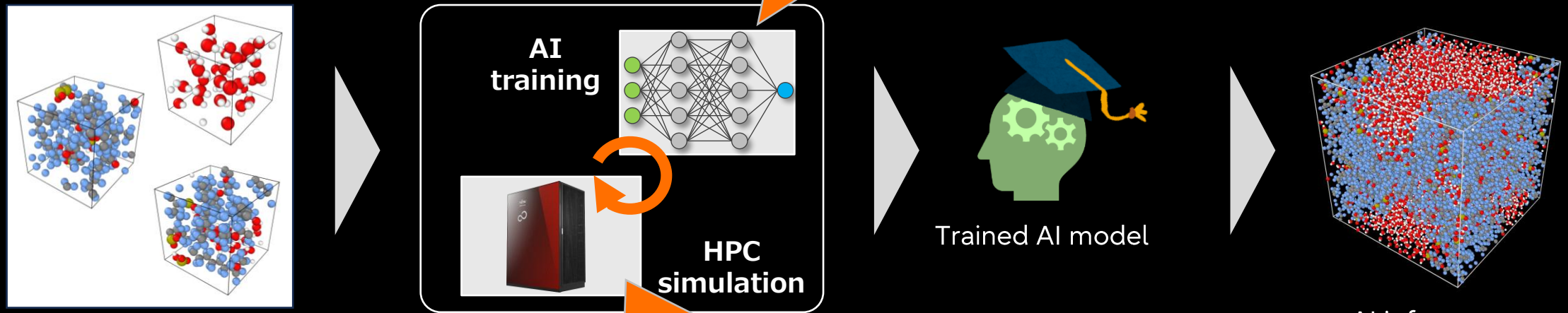
Unique AI training that can accurately represent complex atomic behavior ⇒ **Stable**

Input | **AI model generation** | Output | Simulation



Training data generation by HPC with **our unique data generation method** ⇒ **High accuracy**

Our technologies enable the generation of high-accuracy AI with robust MD stability.

Case Study

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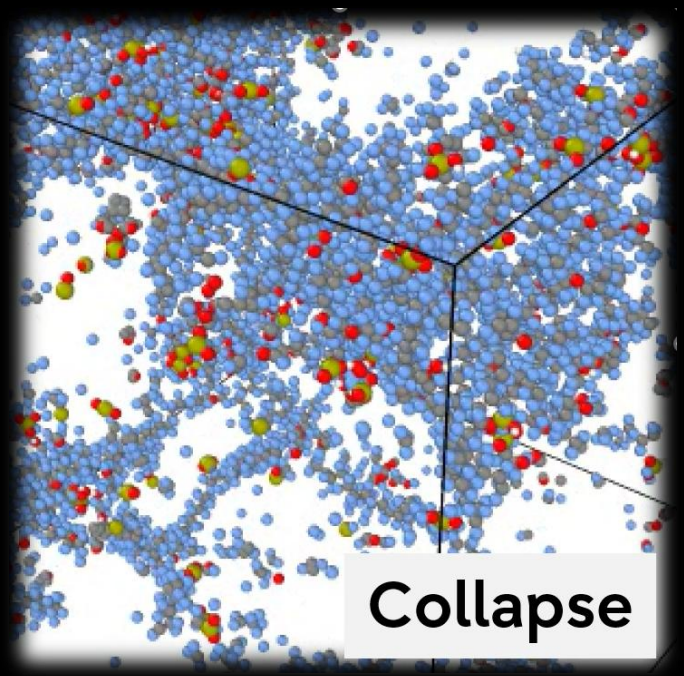
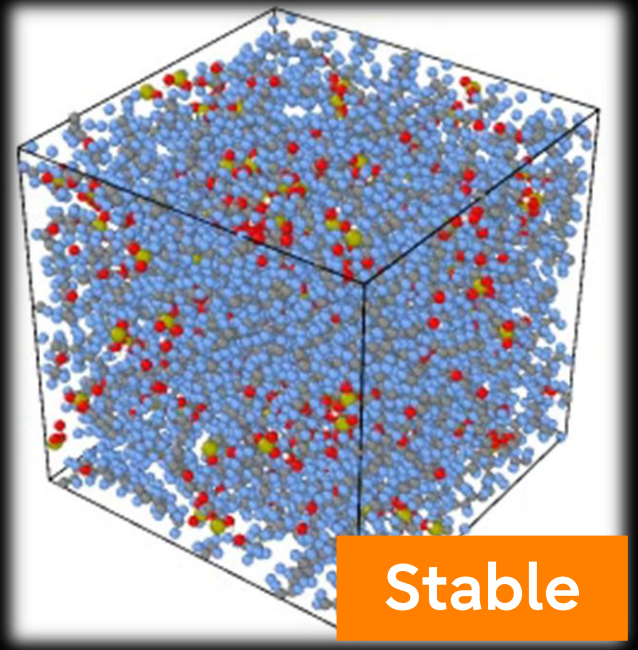
MD Simulation Breakthrough: 20,000 Atoms, 30 ns (60M steps) in 8 Days, cutting simulation time from 800 years with conventional method !

Hydrated Nafion (19,670 atoms)

without our technology



with our technology



Achieved sufficient performance for practical use

10k-atoms : Large enough to design entire devices

10M-steps : Reproducible chemical reactions

1-week : Acceptable computation time

Next frontier:
Simulation-driven materials development

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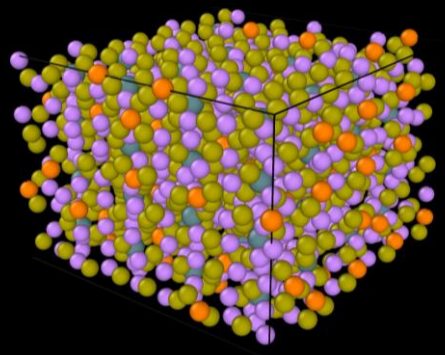
Inorganic

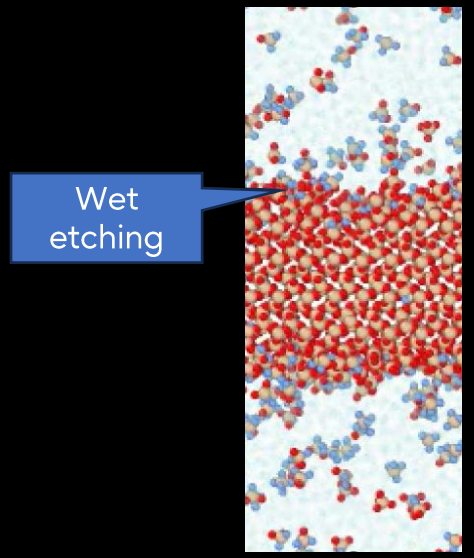
LGPS
(1,600 atoms)



All-solid-state Battery,
Steel, Catalyst

Interface

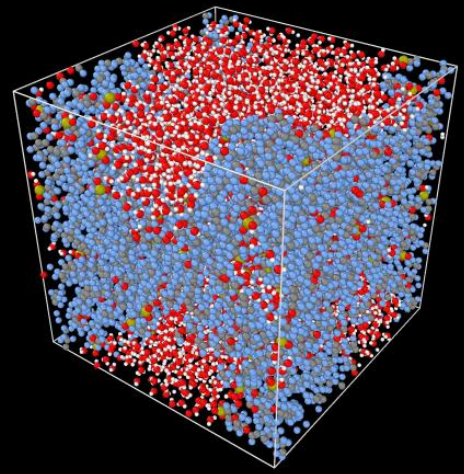
Silica / Hydrofluoric acid
(26,712 atoms)



Semiconductor process,
Semiconductor package,
Li-ion Battery, Adhesive

Organic

Nafion
(19,670 atoms)



Fuel cell, Plastic, Fiber,
Resin, Film

Our ultra-fast & high-accuracy simulation technologies
accelerate simulation-driven materials development across various industries.

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Thank you