HPC Profiles in Leadership

Solving the Mysteries of Electrolytes in Batteries

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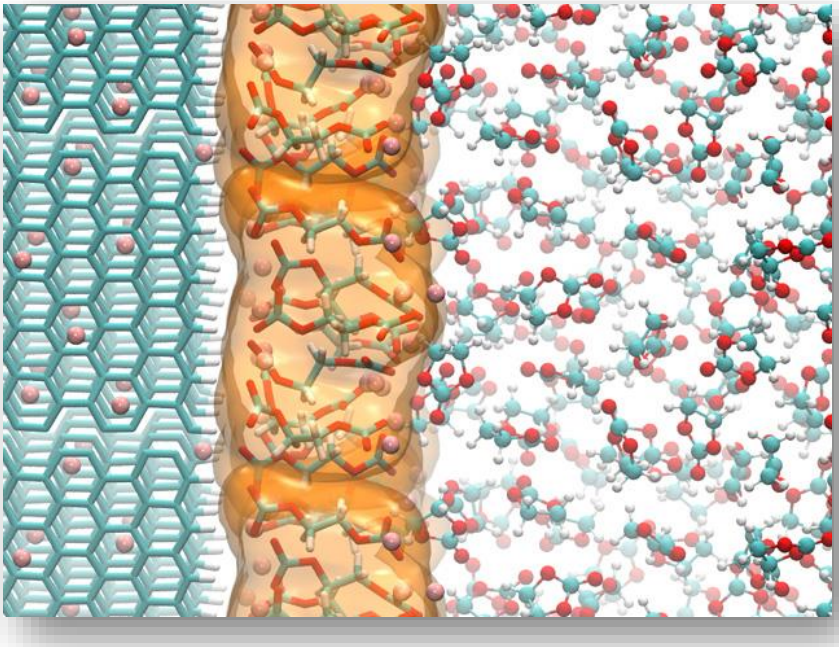
HYPERION RESEARCH OPINION

Scientists affiliated with Japan's National Institute for Material Science (NIMS) Center for Green Research on Energy and Environmental Materials (GREEN) have elucidated long-standing issues associated with electrolytes in lithium-ion batteries that will be essential for the development of more capable next generation batteries. This groundbreaking work was accomplished through large-scale and long-time first-principles simulations that were run on the K computer at Riken's Advanced Institute for Computational Science (AICS). This research, led by Dr. Yoshitaka Tateyama, group leader of the GREEN's Interface Computational Science Group, will provide essential knowledge and novel insights into the control of the battery performance and reliability for their future development.



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SITUATION OVERVIEW

Increasing the performance and efficiency of renewable energy coupled with the realization of zero-emission power supplies are key objectives of the worldwide power research and development community today. To this end, development of larger batteries (including lithium-ion batteries (LIBs)) for electric vehicles etc. has been intensively addressed. However, there remain many problems in achieving higher performance and reliability as well as longer lifetime.

Crucial to resolving these issues are a better understanding of the chemical reaction and interfacial film (e.g. Solid Electrolyte Interphase (SEI)) at electrolyte-electrode interfaces in batteries. Whereas the macroscopic correlation between the electrolyte ingredients (solvent, additive etc.) and characteristics of the battery is somewhat known, the underlying atomistic mechanisms have not been yet fully understood due to the difficulty in in-situ experimental observation.

Dr. Yoshitaka Tateyama and his team used a newly implemented multiple MPI parallelization of the Car-Parrinello Molecular dynamics code, CPMD, for efficient free energy calculations at finite temperature, which allowed researchers to more accurately and efficiently study key reactions. Using this code specifically developed for the K computer, the researchers elucidated the novel mechanisms on solid electrolyte interphase (SEI) films formed at the electrolyte-electrode interfaces as well as the unusual characteristics of superconcentrated electrolytes.

- Their SEI calculations involving electrode, SEI film, and electrolyte needed sufficient size and sampling time that can be only realized by top HPC facilities like the K computer.
- The superconcentrated electrolytes they examined have become very popular as appropriate electrolytes for future batteries, and they are being investigated in many academic institutions and industries.

The K computer, manufactured by Fujitsu and named for the Japanese word Kei (which means 10 quadrillion) allowed for extremely rapid, high-resolution simulations and gave the scientists a greater understanding of some of the complexities surrounding the physical behavior of electrolytes in a lithium-ion battery. Solving some of these long-standing issues is considered essential to the development of the next generation of batteries.

The K computer is based on a distributed memory architecture with over 80,000 computer nodes and is used in a wide range of applications, including drug discovery, climate research, earthquake/tsunami research, weather forecasting, disaster prevention and medical research. Its operating system is based on the Linux kernel, with additional drivers designed to make use of the computer's hardware. With a computation speed of over 8 petaflops, K is now considered the world's eighth-fastest computer.

NIMS defines its mission as developing energy and environment-related materials for realizing energy network systems. Among their projects are materials research for solar cells, solid-state batteries, lithium-air batteries, fuel cells and thermo-electric devices. Computational science and materials informatics for material design and mechanism elucidation are also part of this research. The center includes the Global Research Center for Environment and Energy based on Nano-materials science (GREEN) and NIMS Battery Research Platform.

About Hyperion Research, LLC

Hyperion Research, consisting of the former IDC high performance computing (HPC) analyst team, provides HPC information, analysis, and recommendations based on technology and market trends. Research includes market sizing and forecasting, share tracking, segmentation, technology and related trend analysis, and both user & vendor analysis for multi-user technical server technology used for HPC and HPDA (high performance data analysis). We provide thought leadership and practical guidance for users, vendors and other members of the HPC community by focusing on key market and technology trends across government, industry, commerce, and academia.

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