Researchers raise expectations for commercialization of high-energy-density all-solid-state batteries

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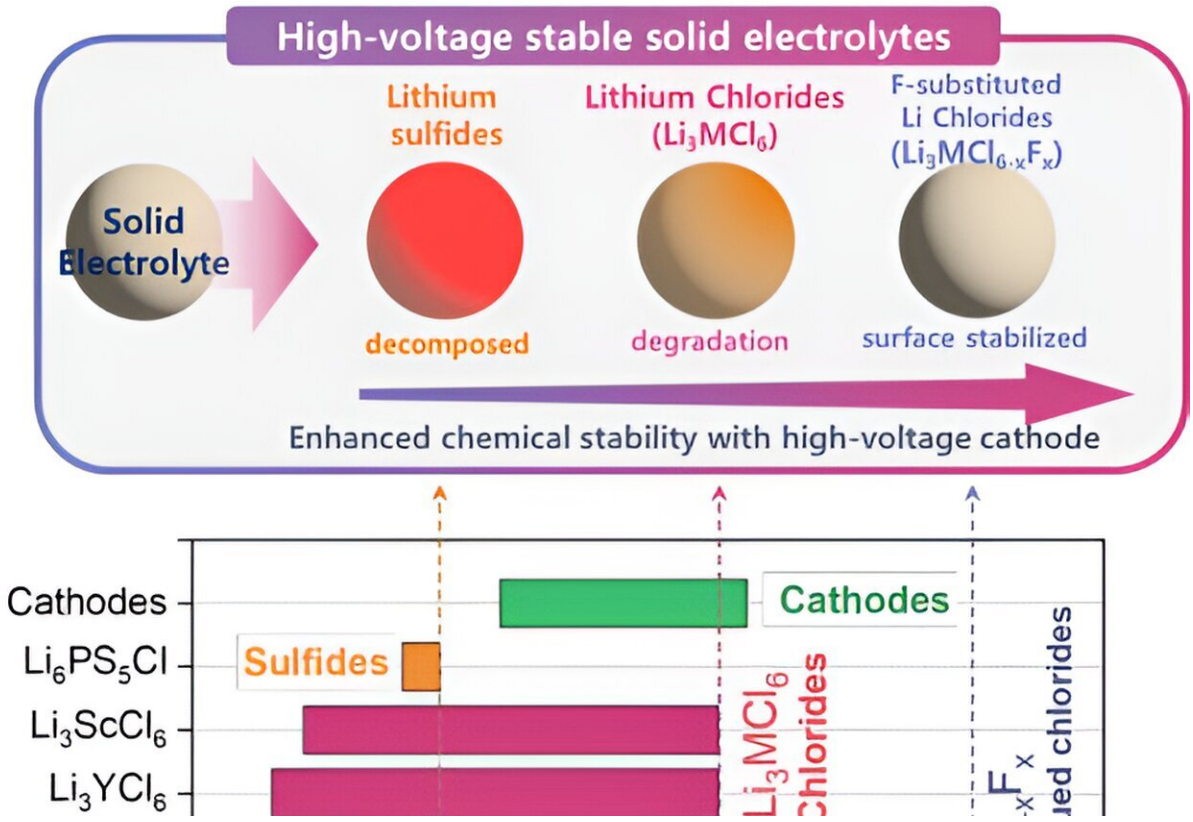


High-voltage stable solid-state electrolytes design strategies. Credit: Korea Institute of Science and Technology

Researchers are actively working on non-flammable solid electrolytes as

a safer alternative to liquid electrolytes commonly found in lithium-ion batteries, which are vulnerable to fires and explosions.

While sulfide-based solid electrolytes exhibit excellent ionic conductivity, their chemical instability with high-voltage cathode materials necessary for high-energy-density batteries has impeded their commercial viability. Consequently, there has been a growing interest in chloride-based solid electrolytes, which are stability in high-voltage conditions due to their strong bonding properties.

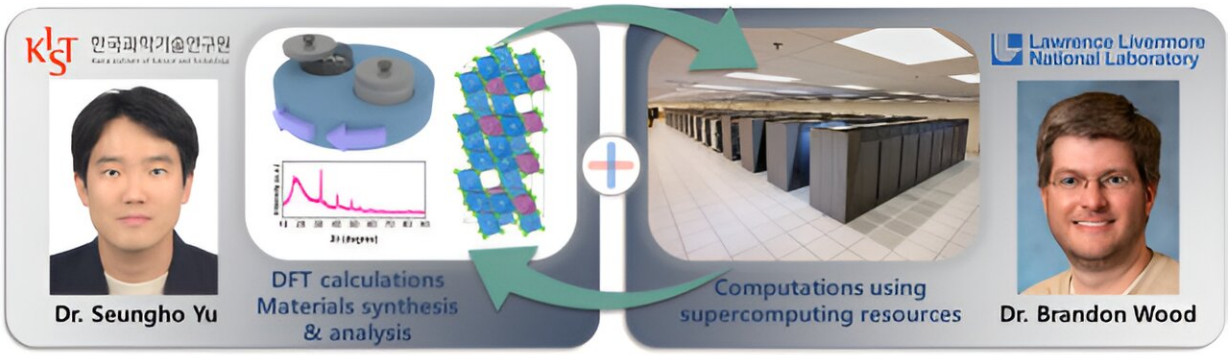
The Korea Institute of Science and Technology announced that a KIST-LLNL joint research team led by Dr. Seungho Yu of the Energy Storage Research Center, Dr. Sang Soo Han of the Computational Science Research Center, and Dr. Brandon Wood of Lawrence Livermore National Laboratory (LLNL) has developed a fluorine substituted high-voltage stable chloride-based solid-state electrolyte through computational science. The work is published in the journal *ACS Energy Letters*.

LLNL is a leading national laboratory under the U.S. National Nuclear Security Administration, known for its excellent supercomputing facilities. Since 2019, KIST and LLNL have been conducting collaborative research in the field of secondary batteries.

To improve the high-voltage stability of chloride-based solid electrolyte (Li_3MCl_6), the research team proposed the optimal composition and design principle of chloride-based solid electrolyte (Li_3MCl_5F) substituted with fluorine (F), which has strong chemical bonding ability.

For the proposed strategy to improve the high-voltage stability of chloride-based solid electrolytes by KIST, LLNL contributed by utilizing their cutting-edge supercomputing resources for calculations and subsequent experimental validations were conducted at KIST. The

collaborative research team adopted a cost-effective and time-saving strategy, wherein computational science guides the initial material design, followed by rigorous laboratory validation.



<KIST-LLNL Collaborative Research on All-Solid-State Batteries>

<2022, 2023 KIST-LLNL joint workshop>

Overview of KIST-LLNL International Cooperation Research. Credit: Korea Institute of Science and Technology

The chloride-based solid electrolyte synthesized based on the design principle proposed by the research team was applied to an all-solid-state battery to evaluate its electrochemical stability under high-voltage conditions.

Impressively, it showed high-voltage stability exceeding 4 V, comparable to that of commercial lithium-ion batteries with liquid electrolytes. Accordingly, fluorine (F)-substituted chloride-based solid electrolytes are expected to replace sulfide-based solid electrolytes that are unstable at high voltages, accelerating the commercialization of all-solid-state batteries.

The Korea-U.S. Joint Research Team will conduct follow-up research on the synthesis process of the material, alongside the optimization of electrode and cell manufacturing processes. These concerted efforts aim to hasten the commercialization of all-solid-state batteries.

In the event of successful commercialization, the U.S.-Korea team will be able to capture the market for solid-state electrolytes, a key component of all-solid-state batteries, in the U.S., one of the largest consumers of secondary batteries such as ESS(Energy Storage System) and electric vehicles.

"This work provides a new design principle for fluorine-substituted high-voltage stable chloride-based solid-state electrolytes, which will accelerate the commercialization of high-energy-density next-generation lithium all-solid-state batteries without fire hazards," said Dr. Seungho Yu of KIST.

"This was a systematic, internationally collaborative study that provided computational science-based design principles for the development of a new solid-state electrolyte and validated them experimentally," said Dr. Brandon Wood of LLNL.

More information: Sooyeon Kim et al, Fluorine-Substituted Lithium Chloride Solid Electrolytes for High-Voltage All-Solid-State Lithium-Ion Batteries, *ACS Energy Letters* (2023). DOI: 10.1021/acsenergylett.3c02307

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