

[1 . Headline](#)

New Light-Element Crystal Framework Paves Way for Safer All-Solid-State Batteries

[2 . Summary Text](#)

All-solid-state lithium batteries promise enhanced safety, but the relatively high weight of conventional oxide solid electrolytes remains a challenge for improving gravimetric energy density. Researchers have discovered that a lightweight crystal framework, $\text{UCr4C4-type RbLi(Li3SiO4)2}$, acts as a high-speed lithium-ion conductor. While defect formation currently limits overall conduction in stoichiometric samples, overcoming this with lithium-rich composition design can unlock its full performance, paving the way for lighter, safer, and faster-charging battery technologies.

[3 . Full Text](#)

Lightweight UCr4C4-Type Crystal Framework Opens New Avenue for Next-Generation All-Solid-State Batteries

TOKYO, JAPAN — All-solid-state lithium batteries using nonflammable solid electrolytes are widely recognized as promising candidates for next-generation energy storage because of their superior safety and fast-charging capability. However, widely studied oxide-based solid electrolytes contain heavy elements such as lanthanum and zirconium, resulting in high densities (e.g., 5.12 g/cm^3) that limit improvements in overall battery gravimetric energy density.

To address this weight challenge, a joint research team led by Nichia Corporation and The University of Electro-Communications (UEC Tokyo) investigated a new solid electrolyte framework composed predominantly of light elements: RbLi(Li3SiO4)2 . Possessing a low theoretical density of 2.74 g/cm^3 , this material adopts a monoclinic UCr4C4-type crystal structure featuring one-dimensional lithium channels.

Combining experimental synthesis with advanced computational simulations—including preferred potential molecular dynamics (PPM-MD) and density functional theory (DFT) calculations—the team uncovered key insights into its ion conduction mechanism:

3D Conduction Network: Although the framework originates from one-dimensional channels along the b-axis, simulations revealed that these channels interconnect to form a three-dimensional lithium transport network. This structure prevents conduction bottlenecks caused by localized crystal defects.

Ultra-Low Migration Barrier: The energy barrier for lithium-ion migration through interstitial sites was determined to be exceptionally low at 0.30 eV . Driven by strong

Coulombic repulsion between adjacent lithium ions, this barrier matches top-performing benchmark solid electrolytes such as Garnet-type $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (0.26 eV).

Clear Design Strategy for Optimization: The researchers identified that in stoichiometric samples, the energy required to form lithium defects (1.26 eV) is significantly higher than the migration barrier, making defect formation the primary rate-limiting factor. Consequently, synthesizing lithium-rich compositions will bypass this bottleneck and unleash the full potential of fast ionic conduction inherent to the framework.

"Our findings demonstrate that the previously overlooked UCr_4C_4 -type framework serves as a highly active platform for lithium-ion conduction," said Prof. Jun Nakamura of UEC Tokyo. "This provides a clear compositional roadmap for developing lightweight, safe, and high-performance all-solid-state batteries".

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Advanced Functional Materials

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