



**SafeBattery  
Safe Lithium-Based Traction  
Batteries**

Programme: COMET – Competence Centers for Excellent Technologies

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## SAFE BATTERIES THROUGH HOMOGENOUS MATERIALS

NEXT-GENERATION BATTERY SYSTEMS ARE EXPECTED TO RELY ON CERAMIC ELECTROLYTES. HOMOGENEOUS CHEMICAL COMPOSITION IS A KEY FACTOR TO GUARANTEE THEIR FULL PERFORMANCE

### Lithium Batteries in Our Daily Life

Batteries are integral components of our daily life. Since their commercialization in the 90s through Sony, the Lithium-ion battery evolved to a highly flexible electrochemical energy storage system in mobile devices and electric vehicles. If we would manage to efficiently store electricity generated from renewable sources such as solar, wind or tidal, we would be able to significantly reduce our dependency on fossil fuels and, thus, to reduce, climate change.

Commercial batteries relying of Li-ions as charge carriers use flammable aprotic liquids to ensure the facile transport of ions between the two electrodes of a battery. In the case of a thermal runaway these liq-

uids represents a major safety issue as toxic decomposition products are produced in relatively large amounts. The use of a solid, ceramic electrolyte, which can be an oxide, hydride or sulfide, is expected to largely reduce the riskiness of a battery.

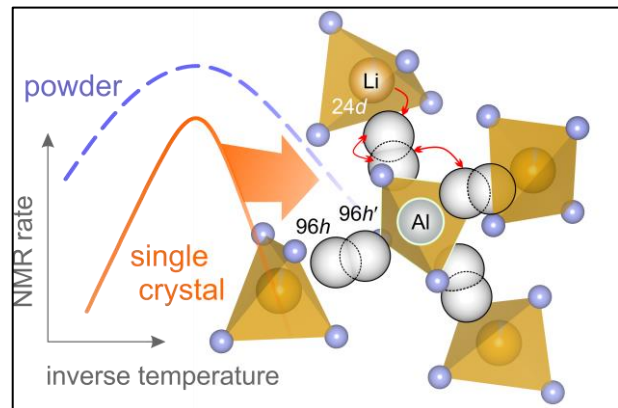
### Paving the Way towards All-Solid-State Batteries

Over the last couple of years, oxide ceramics crystallizing with so-called garnet-type structure were introduced having the potential to herald a new era of all-solid-state battery systems. Provided these ceramics, to which Al-stabilized  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  (Al-LLZO) belongs, show a good compatibility with Li metal and a sufficiently high electrochemical stability, batteries with higher energy densities than commercial liquid-based

## SUCCESS STORY

systems can be developed. Of course, interfacial resistances need to be minimized and ecological production methods have to be evaluated. Quite recently, it turned out that if Al-LLZO is prepared in the form of a polycrystalline sintered ceramic the macroscopic  $\text{Al}^{3+}$  distribution could be inhomogeneous. Hence, regions with lower Al-content offer a lower ionic conductivity than those with optimized composition. Consequently, a non-uniform current density distribution arises which in turn causes safety risks.

Such inhomogeneities, if present in powder samples, make it difficult to elaborate the microscopic transport pathways the Li ions chose to diffuse through the oxide lattice. Such information are, however, urgently needed to understand the reasons behind the very high ion conduction in Al-LLZO. Hence, within the strategic project of Safe Battery we investigated ion dynamics in Al-LLZO single crystals that were grown by the Czochralski method at IKZ in Berlin. We used Lithium nuclear magnetic resonance (NMR) spectroscopy to probe ion dynamics on the atomic length scale. For powder samples, extremely broad rates peaks were obtained and the origin of their shape was unclear for many years. Instead, the homogeneous single crystal shows a narrow peak. We conclude that in the past chemical inhomogeneities hindered us to elaborate the details behind the rapid ion movements in Al-LLZO.



$^7\text{Li}$  NMR relaxation rate peaks of polycrystalline and single crystalline Al-LLZO; these peaks yield information about Li hopping processes in the crystal structure of the garnet. © SafeBattery

### Impact and Effects

The knowledge generated by NMR spectroscopy, when carried out on single-crystalline materials, will greatly help understand the atomistic arrangements needed to achieve very fast Li-ion exchange processes in ceramic electrolytes. These materials should have a very low activation energy for Li-ion transport to ensure that the inner resistance of the battery is kept low also at temperatures well below room temperature. Otherwise charging and discharging a solid-state battery at such low temperatures might be fraught with difficulties.

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- Kreisel Electric, AUT
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