ALISA: Advanced Lithium-Sulfur batteries with ultramicroporous carbons

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Lithium-sulfur (Li-S) batteries hold great promise for high-energy storage, but challenges such as polysulfide dissolution and capacity fading hinder their commercialization. The ALISA project, led by Dr. Alen Vizintin from the National Institute of Chemistry (Slovenia), addresses these issues by optimizing cathode engineering, electrolyte formulations, and nanoporous carbon architectures to enhance battery longevity, rate performance, and energy density.

Recent studies show that sulfur infiltration into nanoporous carbon enables solid-state conversion to Li_2S, effectively preventing polysulfide dissolution. The formation of a cathode-electrolyte interphase (CEI) during cycling stabilizes the electrodes, achieving stability over 1000 cycles. Electrochemical impedance spectroscopy and operando techniques confirm that charge transfer and carbon architecture are crucial for determining battery performance. However, increasing sulfur utilization while maintaining rate capability remains a challenge.

An additional study investigates Li-S conversion pathways using cryo-TEM and machine learning-assisted neutron scattering. It reveals a biphasic discharge structure with nanocrystalline Li_2S embedded in an amorphous Li_2S_x matrix, contradicting the conventional stepwise reduction model. Machine learning analysis supports a disproportion-driven mechanism where Li_2S_2 clusters form first, then aggregate and convert to Li_2S. Cryo-TEM and electron energy loss spectroscopy confirm the presence of multiple sulfur species, underlining the role of amorphous Li_2S_x.

The project's findings emphasize the need for optimized cathode interfaces to control the nucleation and growth of Li_2S. Future efforts will focus on refining cathode-electrolyte interactions, improving material stability, and developing scalable synthesis methods. The successful integration of machine learning highlights its potential for accelerating materials discovery and optimization. Ultimately, ALISA's work advances Li-S battery technology, providing a solid foundation for more efficient, longer-lasting energy storage solutions.

A. Senol Gungor, J.M. von Mentlen, J.G.A. Ruthes, F.J. Garcia-Soriano, S. Drvaric Talian, V. Presser, L. Porcar, A. Vizintin, V. Wood, C. Prehal, Understanding rate and capacity limitations in Li-S batteries based on solid-state sulfur conversion in confinement, ACS Applied Materials & Interfaces 16(49) (2024) 67651-67661.