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IC-MPPE
Integrated Computational Materials Process and Product Engineering.

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Silicon-based anodes in lithium-ion batteries can help to significantly increase the range of electric vehicles. Image: MCL

HOW CAN THE ENERGY DENSITY OF LI-ION BATTERIES BE SIGNIFICANTLY INCREASED?

4D IMAGING TOMOGRAPHY OF LI-ION CELLS REVEALS THE LITHIATION BEHAVIOR OF SILICON: INSIGHTS ENABLE IMPROVED BATTERIES IN TERMS OF RANGE, LIFESPAN, …

The increasing electrification of society requires lithium (Li)-ion batteries (LIBs) with higher energy density, better cycle stability, and longer service life. Achieving these improvements depends heavily on the materials used in the electrodes. Conventional graphite anodes combined with high-energy-density cathodes do not deliver the required performance. New anode material concepts with significantly higher theoretical specific capacity are needed.

Silicon (Si) holds enormous potential as an anode material for LIBs. However, current cells with high silicon content suffer from long-term stability issues. One major problem is the significant volume expansion of silicon during lithium-ion uptake. Despite advances in electrochemical understanding, the effects of mechanical processes associated with charging and discharging, both at the electrode level and within individual silicon particles, remain poorly understood. In particular, a combined understanding of electrochemical and mechanical mechanisms could enable substantial improvements in cycle stability and lifetime.

According to previous understanding, silicon was thought to lithiate via a so-called two-phase core-shell mechanism. In this process, the outer region of the silicon transforms into a Li–Si compound, while the inner core remains as silicon. These insights are mainly based on in situ transmission electron

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microscopy experiments. However, such studies are limited because they are conducted on idealized cell systems that do not represent realistic anode microstructures consisting of many silicon particles embedded in a porous matrix with binder domains.

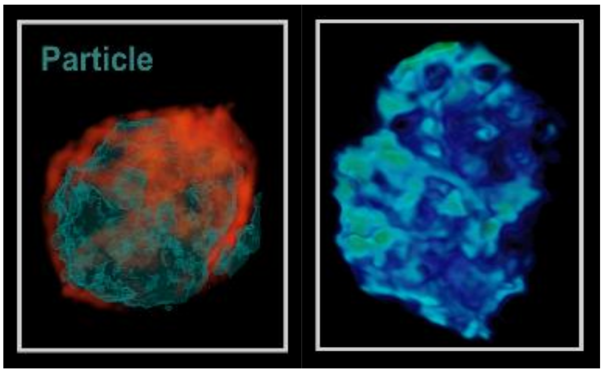
Impact and Outlook

The published work sheds light on the interplay between mechanical and chemical mechanisms during silicon lithiation, from the electrode scale down to individual particles, using high-resolution 4D synchrotron tomography. It demonstrates that the previously assumed core-shell lithiation model represents only part of the reality in non-ideal electrodes. Many silicon particles do not follow this model but instead exhibit more complex lithiation behavior that also involves the particle interior.

These multi-scale 4D investigations show that electrode stability and battery lifetime are influenced not only by silicon's volume expansion - as previously assumed - but also significantly by local stress concentrations and the electrode's microstructure.

These findings provide key insights for future improvements in cycle stability and lifespan.

This project represents a breakthrough in battery research. It has been recognized by the journal EES Batteries as a research highlight and selected as a HOT Paper 2026.



On the left, the lithiation (red) evenly surrounds the silicon particle (cyan), while the complex pattern on the right (blue) accelerates battery aging.

M. Häusler et al. Bridging particle-scale lithiation mechanisms and macroscopic performance in high-energy density Si anodes via time-resolved full 3D visualisation. EES Batteries (2026).

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