

Solid state sUlfide Based LI-MEtal batteries for EV applications

Deliverable 7.2 Mechanism of Li transport and dendrite formation in all solid battery

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Publishable summary

Work Package 7 of the SUBLIME project focuses on driving the iterative development of SUBLIME material and cell sulphide solid-state battery technology through physics-based multiscale modeling. This report discusses Li diffusion in bulk argyrodite and complex interface structures. The Nudge Elastic Band (NEB) approach is used that calculates the Minimum Energy Path (MEP). Further, the diffusion coefficient is calculated using this barrier energy through the Kinetic Monte Carlo code. The diffusion coefficient obtained is used as an input parameter for modeling Li dendrites through the phase-field approach. Li dendrites are modeled to understand their effects at different operating temperatures and current densities. Force field parameters are optimized for Li₂S coating on Li anode to investigate the Li diffusion further. The main conclusions are summarised at the end of the report.