

All-Solid-State Cells – Dynamics and Interfacial Processes

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Recently, solid electrolytes (SEs) have experienced a growing interest as potential future components of safe next-generation high voltage batteries. One key challenge of all-solid-state battery (ASSB) cells is the high interfacial resistance. Reasons for the large charge transfer resistances are still subject to scientific discussion. To advance ASSB design, fundamental knowledge of the underlying interfacial processes is essential.

In this contribution, we investigate the processes in ASSB cells by continuum modelling and numerical simulations. The physical model extends the rigorously derived transport model for SEs [1] to ASSBs and further includes the concentration dependence of the dielectric SE properties. The framework describes space charge layer (SCL) formation and self-consistent charge transport in the SE by Poisson's equation coupled to a cation continuity equation with a generalized molar cation flux. Particular attention is driven to the connection between measured material parameters and material parameters entering the equation system. Furthermore, the electric SCLs in the electrodes are approximated giving rise to effective interfaces and respective conditions coupling the electrodes to the SE. The charge transfer process at the electrified electrode-SE interface given by a defect reaction mechanism is modelled via a Butler-Volmer like approach. Based on this hybrid-approach computational results are presented and compared to experiments.

[1]S. Braun, C. Yada, A. Latz, Thermodynamically Consistent Model for Space-Charge-Layer Formation in a Solid Electrolyte, J. Phys. Chem. C. 119 (2015) 22249–22746.