# Thermodynamically Consistent Modelling and Simulation of Space-Charge Layers in Solid Electrolytes

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Due to increasing efforts in the development of ecological friendly automotives, all-solid-state batteries have experienced a growing interest in the recent years and have become one of the central issues of current research activities. Still facing with problems such as large interfacial resistances and low power density, theory based modeling can help to understand the underlying processes on the microscopic and mesoscopic scale and thus deliver valuable information in order to support experiments and battery design. In [1] a thermodynamic consistent model was formulated by Braun et al. that is capable of describing space-charge layer (SCL) formation in solid electrolytes (SEs) on basic physical laws comprising electrodynamics, thermodynamics and classical mechanics, only. The transport mechanisms in the solid are described via mobile cations and Schottky defects moving through a stationary anion lattice resulting in one consistent ion flux. Based on this model we numerically simulate the transient processes within SEs. The entire set of equations is discretized via the finite volume method and solved numerically by applying a Newton type method to the fully coupled, implicit PDE system. The results presented encompass a material study for different dielectric susceptibilities and a variation of the cell thickness showing both a significant influence on the spatial extension of SCLs. Furthermore, boundary modifications using $BaTiO_3$ nanoparticles, motivated by Yada et al. [2], have been implemented revealing “lithium-ion-pathways” found in experimental data.

[1] S. Braun, C. Yada, A. Latz, *A Thermodynamically Consistent Model for Space-Charge-Layer Formation in a Solid Electrolyte,* J. Phys. Chem. C, 2015, 119 (39), pp 22281-22288

[2] Yada, C., Ohmori, A., Ide, K., Yamasaki, H., Kato, T., Saito, T., Sagane, F., Iriyama, Y. (2014). *Dielectric Modification of 5V-Class Cathodes for High-Voltage All-Solid-State Lithium Batteries.* Adv. Energy Mater., 4*: 1301416. doi: 10.1002/aenm.201301416*