

SOLIDBAT

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Digital Tool For SSB Cell Design

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1 EXECUTIVE AND PUBLIC SUMMARY

This report describes part of the activities of Work Package 2 of the SOLIDBAT project. It provides the implementation of a digital tool for solid-state battery cell design as well as an extensive set of molecular modelling results.

Based on the ISEA Cell & Pack Database (ICPD) [1], developed by RWTH Aachen University, the simulation of virtual solid-state battery cells is showcased for the small (1 Ah) and large (5 Ah) cell under development within the SOLIDBAT project. The results of a multi-million parameter study for both cell types are presented and analyzed. This report shows the tremendous power of using the ICPD to simulate millions of possible virtual cell designs. These multi-million parameter variations enable a detailed investigation of dependencies of outputs, such as capacity or energy densities, on cell parameters. The analysis is supported by the interactive data viewer presented in this report, which allows users to explore all possible combinations within certain boundary conditions.

Furthermore, the computational screening and characterization of different electrolyte components was conducted through density functional theory (DFT) and molecular dynamics (MD) simulations. Here, CIC energiGUNE presents a quantitative framework to predict the electrochemical stability and ionic transport properties of candidate formulations. These activities provided critical insights into the structure-property relationships of multi-component electrolytes, identifying promising diluents and crosslinkers. The identified candidates bridge the gap between molecular design and high-performance electrolyte development.

[1] M. Kuipers, S. Bihn, M. Junker, and D. U. Sauer, "Development of a cell design environment for bottom-up estimation of performance parameters for lithium-ion batteries and virtual cell design – ISEA Cell & Pack Database (ICPD)," Journal of Energy Storage, vol. 72, p. 108396, Nov. 2023, doi: 10.1016/j.est.2023.108396



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