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Strongly improved, highly performant and safe all solid-state batteries for  
electric vehicles.

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**SAFELiMOVE – Deliverable Report**

**D9.1 – Interface Modelling**

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## Publishable summary

This report describes the activities carried out within the Task 9.1 and Task 9.2 of Work Package 9 in SAFELiMOVE project. It provides a framework for the modelling and design optimization of solid electrolyte lithium metal batteries. Starting from the standard P2D electrochemical model, WP9 has analyzed and included the most relevant phenomena of solid electrolyte batteries to provide tools to guide the material and cell development.

The adaptation of the standard P2D to lithium-metal solid electrolyte cells has been discussed highlighting the main limitations of the model for the materials used in this project. These are:

- The transport of ions in a composite electrolyte
- The complex kinetics and dendrite growth at the lithium metal
- The mechanical issues of the solid electrolyte that can lead to interfacial contact problems

These limitations have been studied in detail separately and several methods and approaches to account for the relevant phenomena have been proposed.

This deliverable D9.1 resumes the work done within WP9 Tasks 9.1 and 9.2, including the adaptation of the P2D model to a lithium metal solid electrolyte cell, the analysis on how the composition of the electrolyte affects its conductivity by 3- fold approach in modelling, the study on how to include the mechanical problem in the P2D model, the analysis of the dendrite growth using phase-field models and the sensitivity analysis of the main parameters of the P2D model.

Furthermore, this report aims to provide a baseline for the definition of the models used in SAFELiMOVE project and a guide for the development of materials that lead to increased cell performance.

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