

**EUROPEAN COMMISSION**

HORIZON 2020 PROGRAMME - TOPIC H2020-LC-BAT-2020  
Sodium-Ion and sodium Metal Batteries for efficient and sustainable  
next-generation energy storage

GRANT AGREEMENT No. 963542



SIMBA – Deliverable Report

<< D3.3 – Quantification of Na<sup>+</sup> transfer at  
electrode/electrolyte interfaces >>

## Publishable summary

A deep understanding of the interaction between the solid-state electrolyte and the electrodes is essential for the development of an efficient all-solid-state battery. Stable interfaces with the anode and cathode will ensure inherent safety and will ultimately lead to the extended lifetime of the battery. Highly efficient electrolyte/electrode interfaces through an intimate solid-solid contact are a key feature of solid-state batteries. One of the key challenges toward high-performance solid-state batteries is the large impedance posed by the electrode-electrolyte interface. However, a direct assessment of the charge transport across realistic electrode-electrolyte interfaces is tedious. The lack of understanding of the processes at the interfaces between the electrolyte and the electrodes is one of the biggest challenges for sodium ion batteries.

In this report we list and discuss in detail the possible ways of the evaluation of the diffusion coefficients of sodium in the electrode (both cathode and anode), electrolyte and well as the charge transfer resistances across the electrode/electrolyte interface. This description provides a “mode d’emploi” (detailed guideline) on how to determine a charge transfer across the cathode/electrolyte interface. Accordingly, the methodology of experimental and modelling approaches allowing to assess the charge transfer properties of the interface is addressed in line with the limits of the technique. The detailed description of the evaluation of the sodium ion transfer in the interface using NMR spectroscopy and single particle measurements is presented in line with a determination of sodium transport using molecular dynamic simulation and DFT calculations. Summarizing, here we aim to provide a trend-setting toolbox allowing to characterize and to improve the charge transfer/ion mobility in the electrode/electrolyte interface.

Please keep in mind that a detailed didactic description of a methodology proposed in this document in line with scientific basics for the discussed techniques has been presented in Deliverable 3.1 and 3.2 and is not in the focus of a present deliverable.

## Appendix B - Acknowledgement

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| 2  | UU      | UPPSALA UNIVERSITET  |
| 3  | UBham   | THE UNIVERSITY OF BIRMINGHAM   |
| 4  | WMG     | THE UNIVERSITY OF WARWICK  |
| 5  | KIT     | KARLSRUHER INSTITUT FUER TECHNOLOGIE   |
| 6  | CEA     | COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES   |
| 7  | IFE     | INSTITUTT FOR ENERGITEKNIKK  |
| 8  | SAS     | USTAV ANORGANICKEJ CHEMIE SLOVENSKA AKADEMIA VIED (Institute of Inorganic Chemistry, Slovak Academy of Sciences) |
| 9  | FHG     | FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V.  |
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