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SIMBA – Deliverable Report

<< D3.5 – Selective NMR data and structural information for the new Na-containing materials >>

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Publishable summary

The identification of structure moieties in components (electrodes, electrolytes, etc.) of sodium/sodium ion battery systems is a challenging task due to the high degree of disorder in the materials that require appropriate analytical techniques allowing the detection of local structures. Solid-state NMR spectroscopy has been identified as a powerful tool to address this quest. While ^{23}Na in-situ solid-state NMR of sodium/sodium ion cells, evaluated already in deliverable D3.2, allows to monitor structural changes in cells during galvanostatic cycling processes and gives an overall picture on what happens structurally in a cell during charging and discharging, in many cases it suffers from its low resolution. To overcome this issue an analysis of the single components (electrodes, electrolytes, etc.) of the sodium/sodium ion cell is required that can be done by high spinning high resolution ^{23}Na ex-situ MAS NMR. Moreover, to support the interpretation of NMR data in terms of structure moieties, quantum chemical calculations are mandatory that can be done at the DFT level of theory on model compounds mimicking the suggested structure moieties.

The successful preparation of an electrochemical cell containing Na|$NaPF_6$|SiCN for solid-state NMR studies is presented. The obtained ^{23}Na in-situ NMR spectra allow to inspect structural changes in the overall cell system. Following disassembling of the cell and analysis of local structure occurring in SiCN electrode materials by ^{23}Na ex-situ MAS NMR delivers insights into the sodium storage process in this cell.

Finally, a combined experimental/theoretical approach is presented that allows a more detailed analysis of carbon and silicon-containing sites in SiCO ceramics which in the future can be transferred also to sodium-containing sites in electrode materials.

Appendix A – Acknowledgement

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Project partners:

#	Partner	Partner Full Name
1	TUDa	TECHNISCHE UNIVERSITAT DARMSTADT
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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13	SAFT	SAFT
14	Altris	ALTRIS AB
15	Recupyl	TES RECUPYL SAS
16	UNR	UNIRESEARCH BV

Appendix B – Disclaimer/Acknowledgement

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