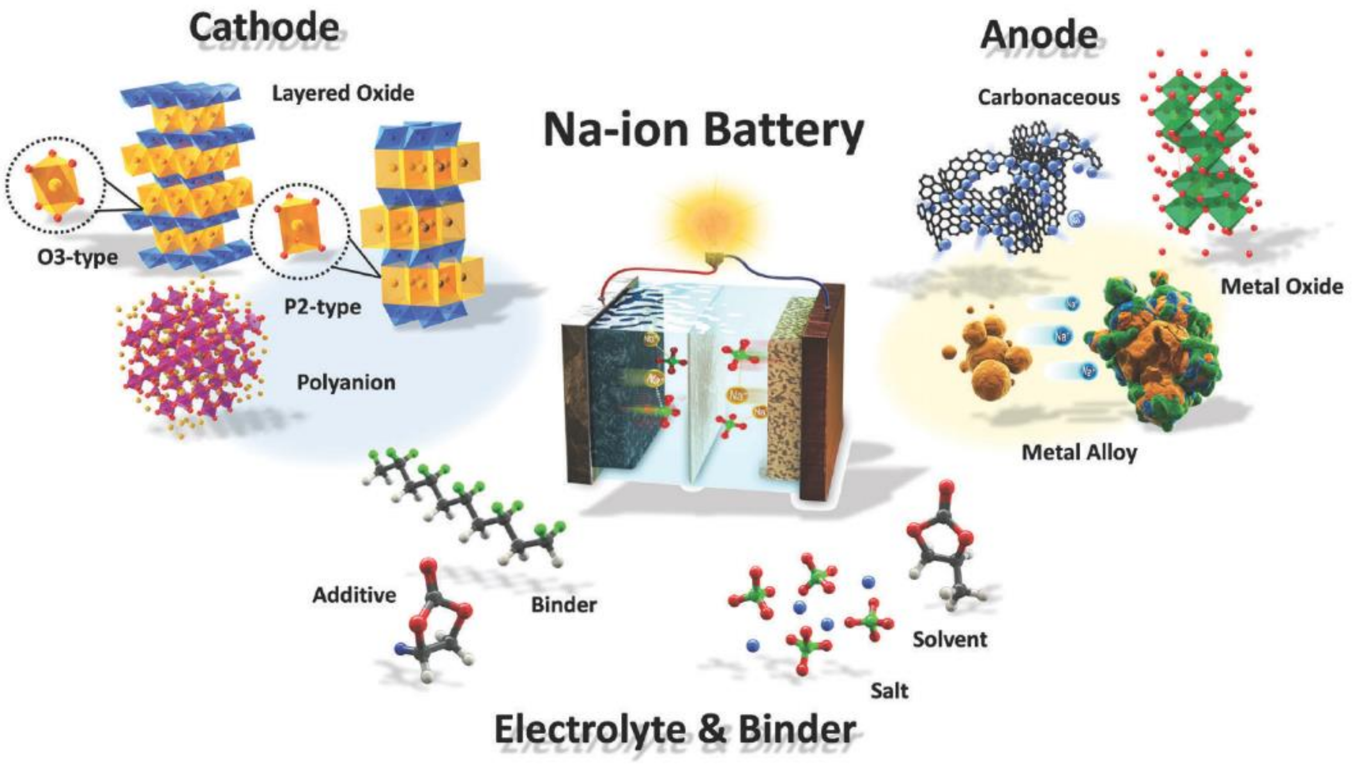
Leibniz Institute for Solid State and Materials Research Dresden

TAC Meeting

Björn Pohle 17.02.2022

Determination of battery parameters

- OCV + temperature dependency
- Particle morphology
- Diffusion coefficient



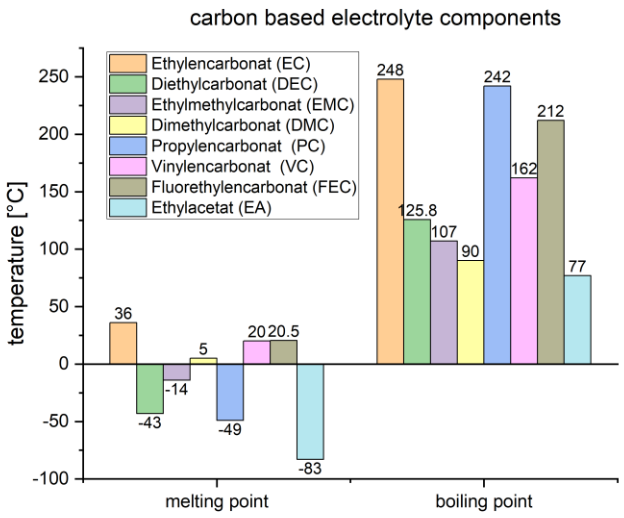
- OCV + temperature dependency
- Particle morphology
- Diffusion coefficient

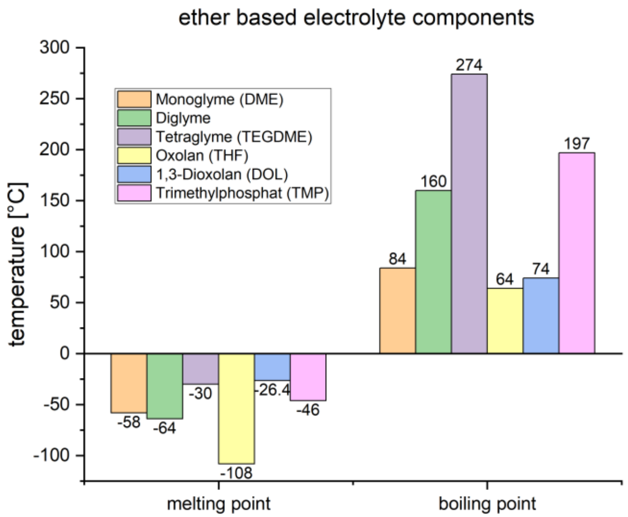
- Conductivity
- Transport number
- Diffusion coefficient
- Thermodynamic Factors

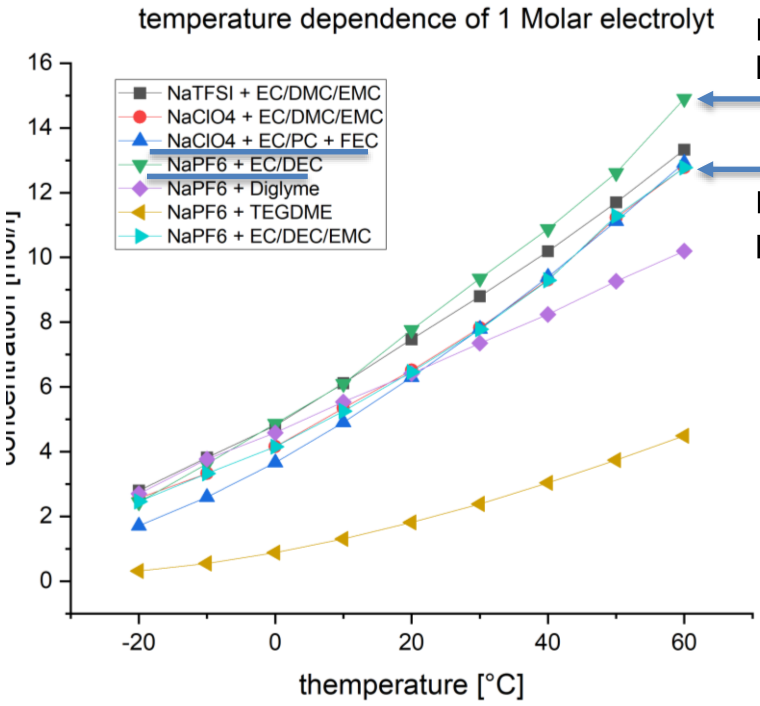
Picture: Chem. Soc. Rev., 2017,46, 3529-3614

Selection of the electrolyte

- Large number of components possible, there are currently 2 typical representatives, typically Ether- and Carbonate-based systems
- Possible usable range for the application between -20 to 60°C
- Melting point of sodium 97,8°C







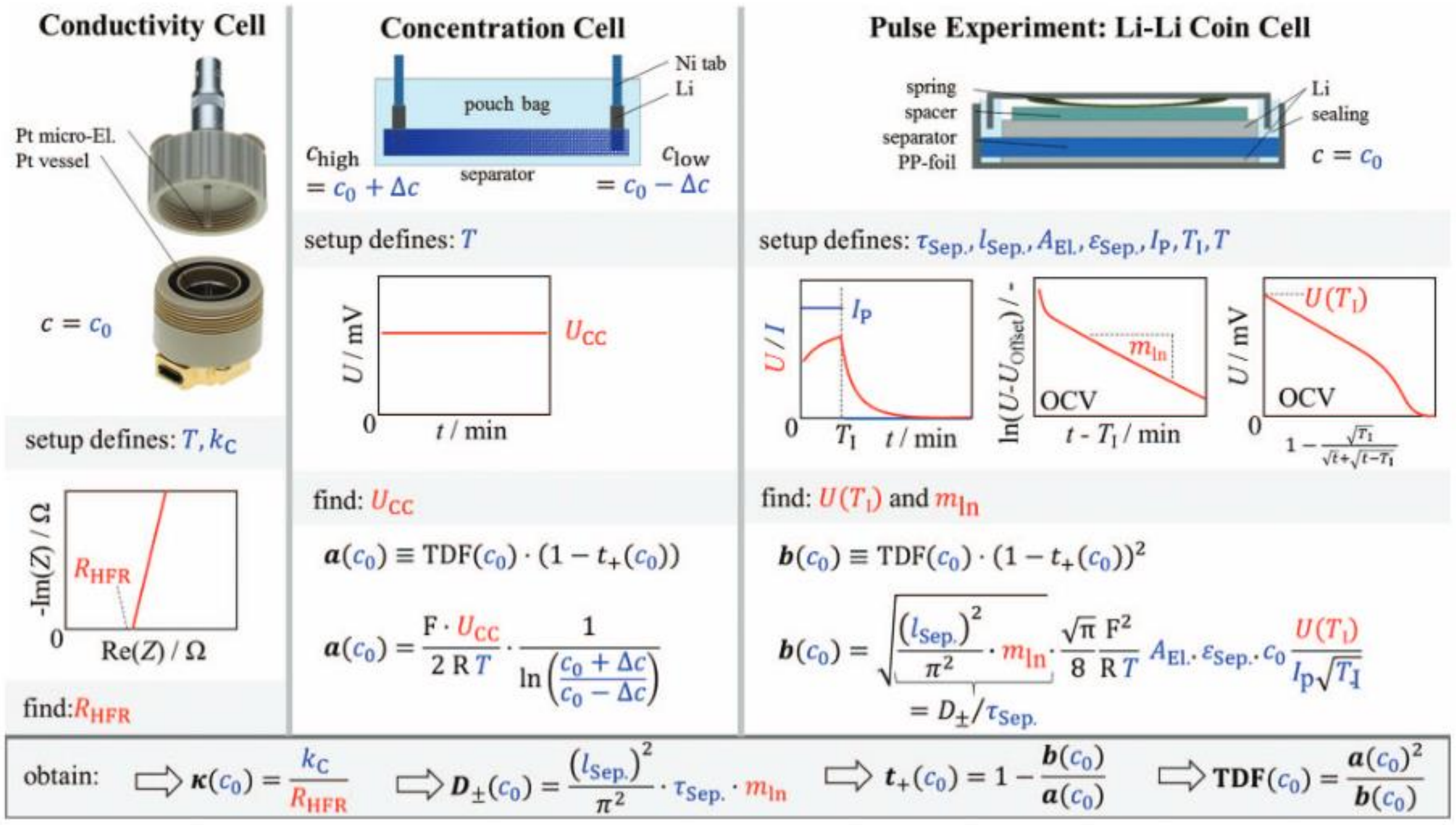
Equivalent to lithium batteries

Most used in publications

Analysis of literature data

Calculation of electrolyte parameter

- Modification of the origin setup with the complete RHD instruments setup
- Sodium is more reactive for contaminate
- All measurements is execute in the glovebox

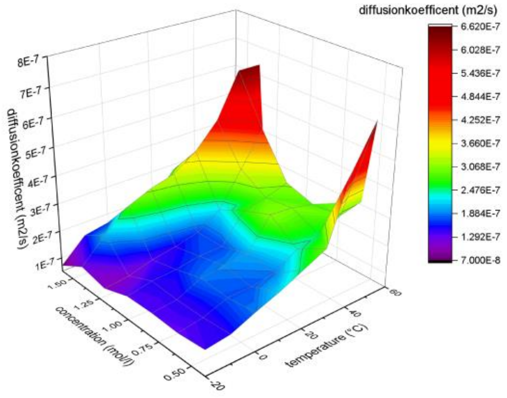


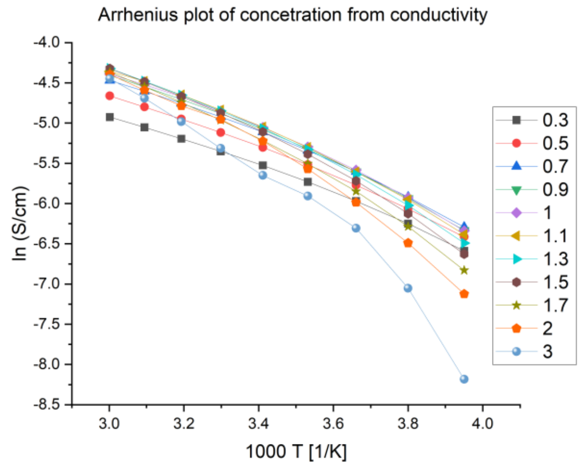
finish 1 electrolyte | finish 1 electrolyte | In process 1 electrolyte

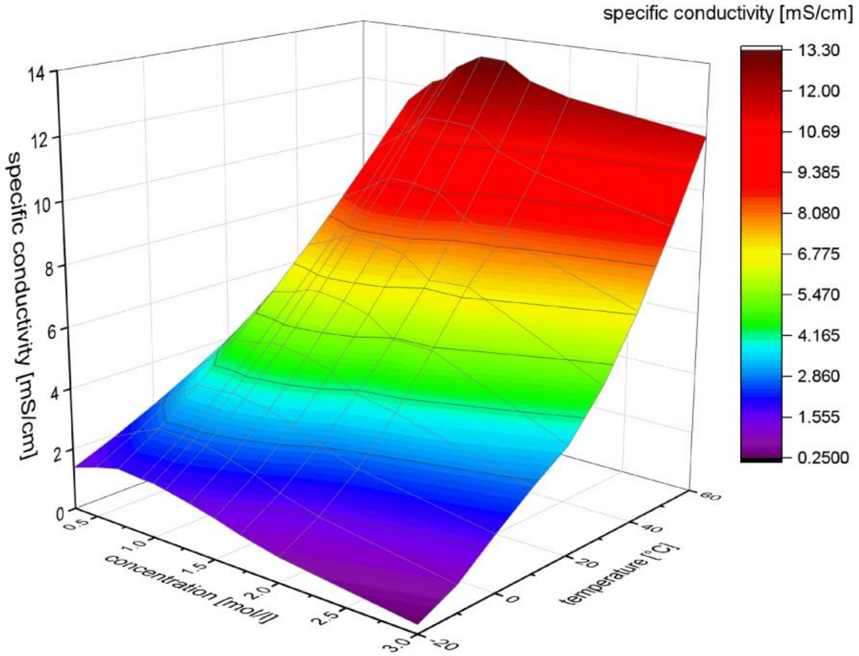
Journal of The Electrochemical Society, 166 (14) A3079-A3097 (2019)
https://www.rhd-instruments.de

Characterisation electrolytes

- measurement setup (fluid cell, symmetric cell, concentration cell)
- electrolyte contains 1M $NaClO_4$ in EC/PC 1:1 + 5 % FEC
- Temperature range between -20 to 60 °C
- Determination of the parameters with EIS / GITT / OCV
  - Specific conductivity - EIS measurement
  - Diffusion coefficient - GITT
  - Transport number - Polarisation

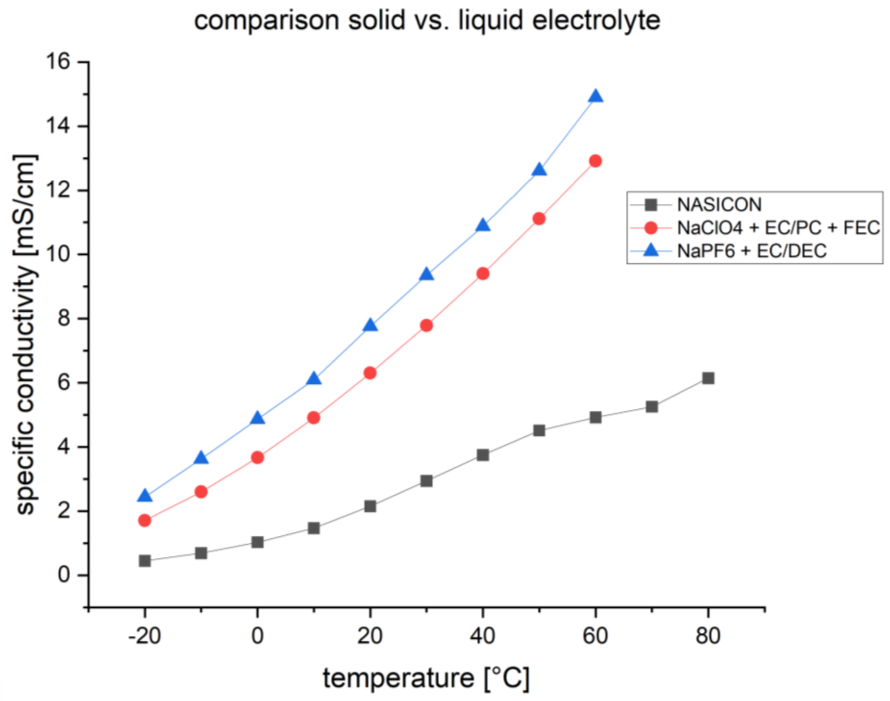






Next steps for the electrolyte parameter

- Carbonate-based electrolytes have a lower stability in sodium cells in comparison to lithium cells → determination the parameter for Ether-based systems with Diglyme
- Finish the parameters calculation for the EC/PC + FEC setup, and a solid-state electrolyte with the NASICON-structure
- Creation of a materials database for the electrolytes

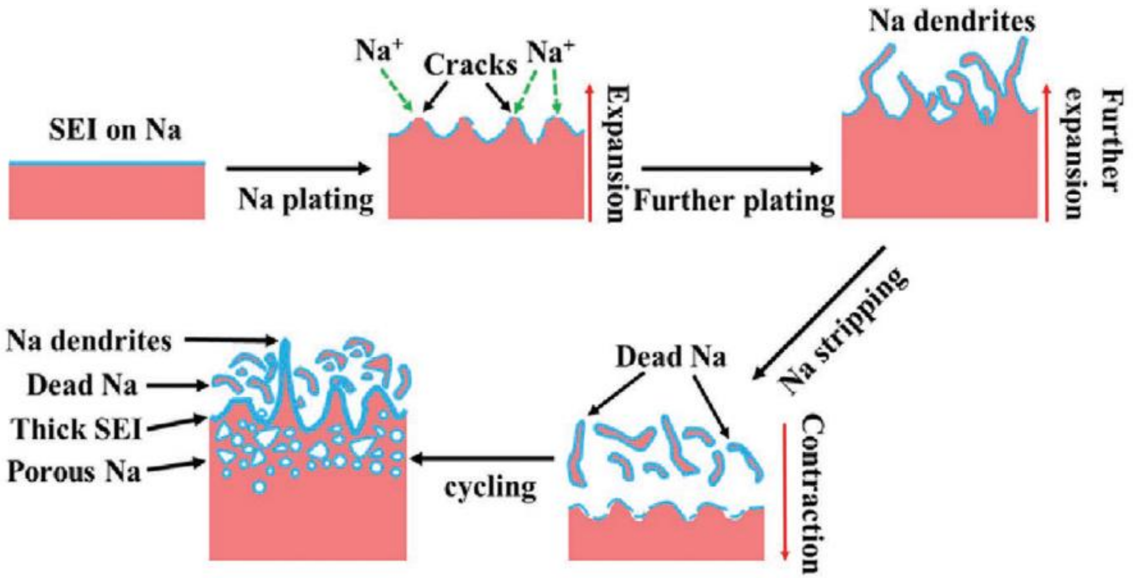


Anode characterisation

- Stability of a pure metal anode is low without any modification of the surface and not direct usable, this effect is not pronounced in lithium cells
- During cycling, Na dendrites are growing and destroy the surface → capacity reduction

- Opportunities of the modification
  - Thin artificial SEI layers or coatings
  - 2D or 3D Anode structures
  - Electrolyte modification

→ The characterisation without any modification is possible, but a fast capacity loss is observed

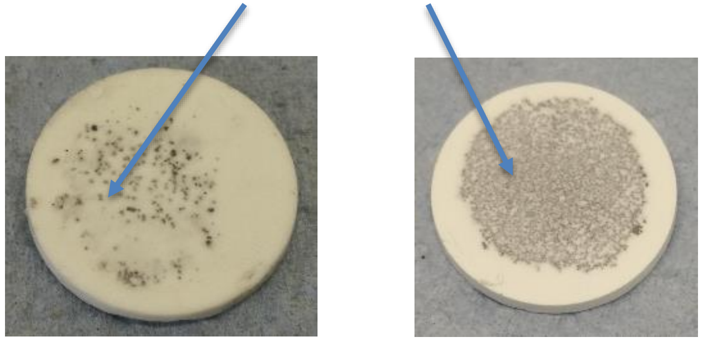


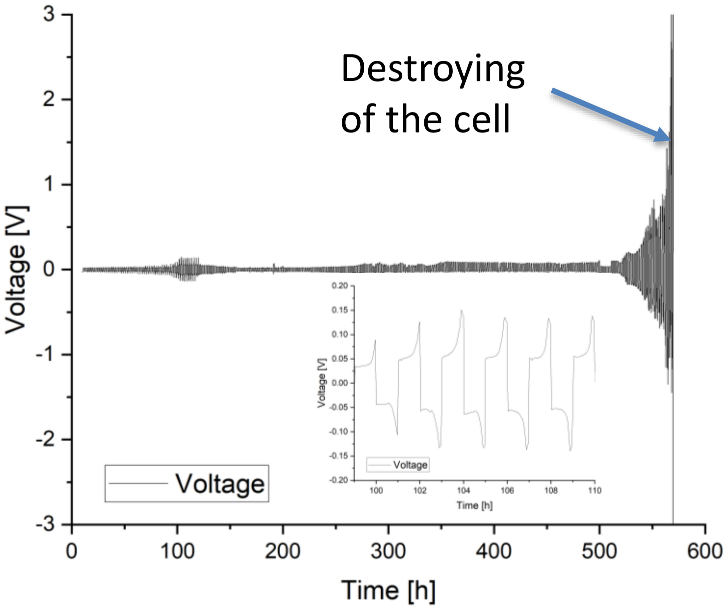
https://doi.org/10.1002/adfm.202004891

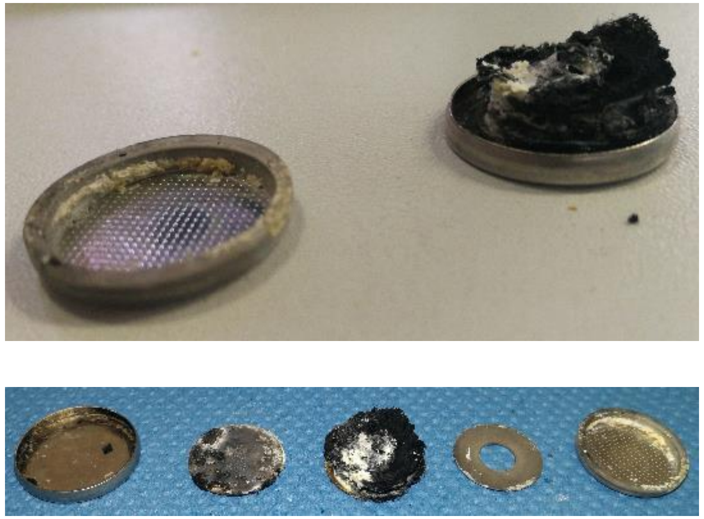
Effect of the metal dendrites

- Dependency of the dendrite growth on temperature, current density, concentration of the electrolyte and the current density
- Without dendrite growth preventing, destroying of the cell with a short circuit or fire / explosion is the result
- The change from a liquid to solid-state electrolyte increases the safety, but the risk for dendrites as well

Dendrites inside
the NASICON pellet





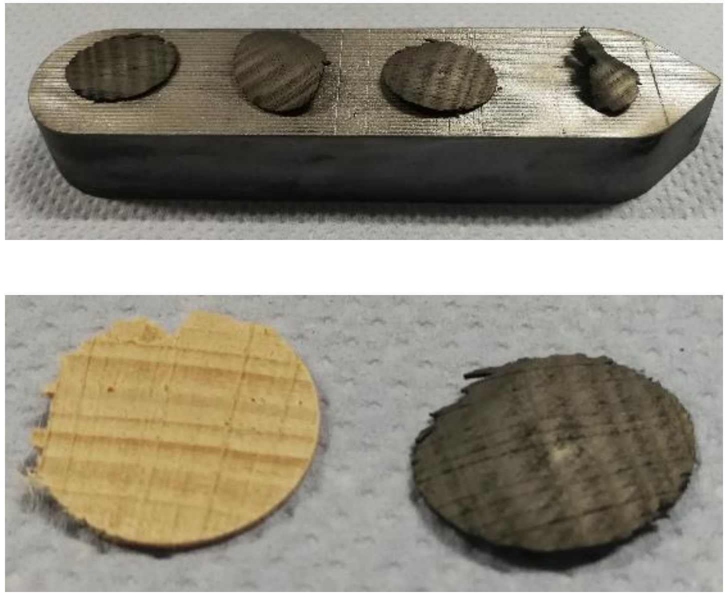


Destroyed coin cell because of a short circuit

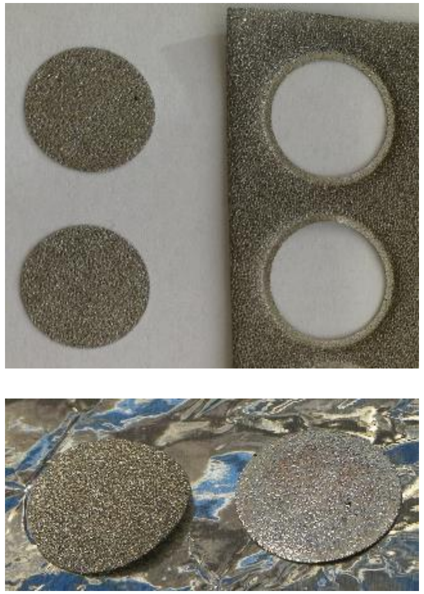
Anode Modification

- different possible ways for protection of the sodium metal anode
- the target from 2D / 3D material is an defined structure for the infiltrated sodium
- with the coated layer or films, a formed protection barrier or alloy at the surface is created

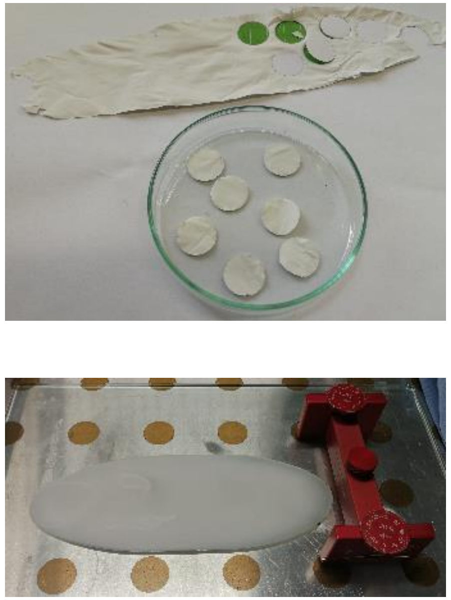
Carbonized MOF structure



Carbonized wood (L original, R carbonized)



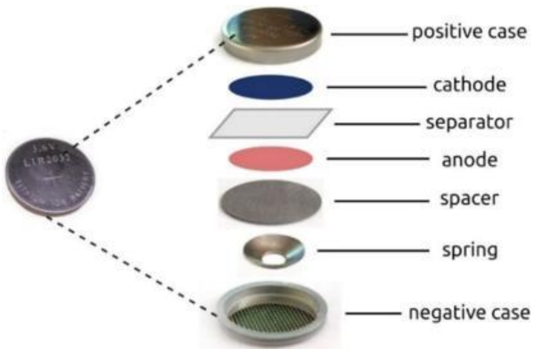
Nickel foam(L without, R with Sodium)

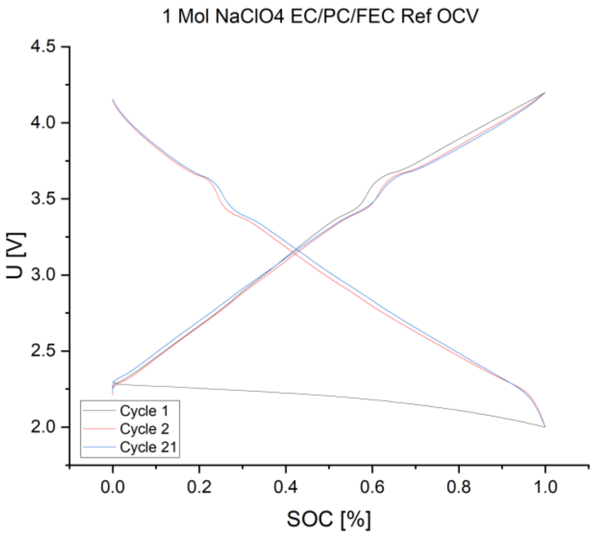


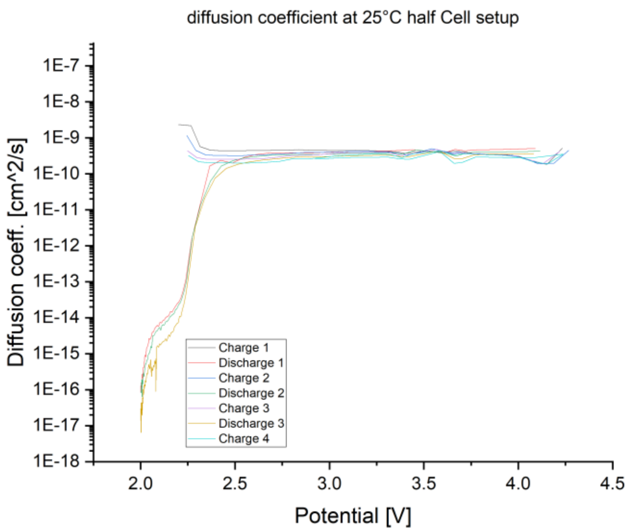
thin PVDF-Al_2O_3 film

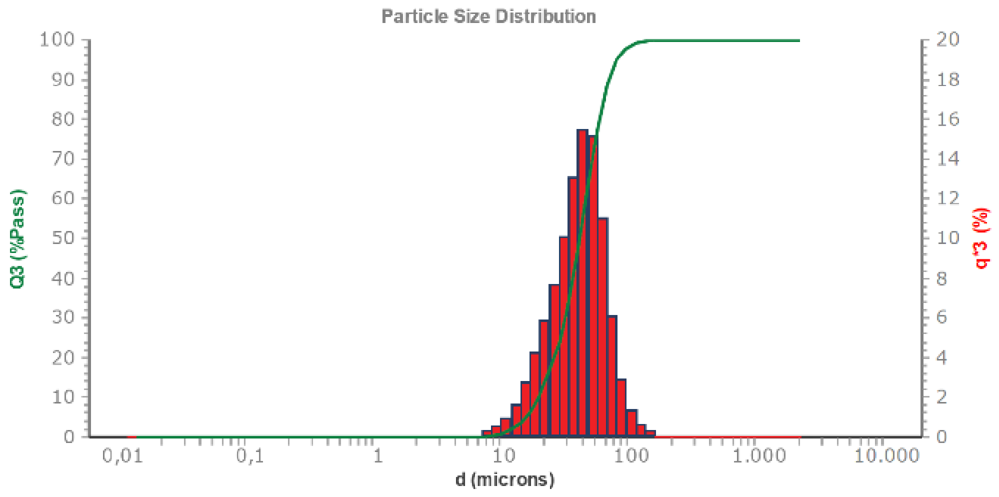
Cathode characterisation

- Determination of the electrochemical parameters with coin cells 2025
- Self-synthesized stable cathode material $Na_xCo_{0.8}Ti_{0.2}O_2$ with a good specific capacity of max. 120 mAh/g
- Measurement of the materials performance at 0°C, 25°C, 40°C and 60 °C
- Publication is in preparation







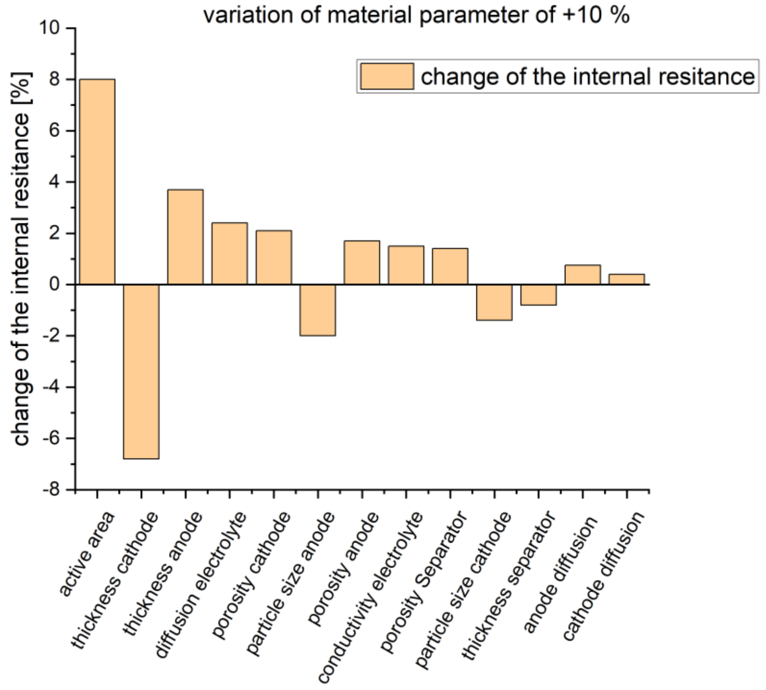


Next Steps

- To finish the characterisation of anode and cathode materials
- To define the anode modification with good stability of the anode
- To create the materials database for electrode materials/ electrolytes

- Build up an p2d sodium batteries model
- validate the model with real measurements

- To finish two publications about the cathode materials



Example for simulations from past work

Thank you for your attention

Optional informations

Characterisation of the separator material (Whatman GF/D)

thickness	0.025	cm
density	2.23	g/cm^3
porosity	94.49	%
tortuosity	2.154	
McMullin numbers	2.28