Model-based identification of high energy density solid-state lithium-ion batteries with hybrid electrolytes

S. Toghyani[1], F. Baakes[1], W. Cistjakov[2], N. Zhang[3], H. Kühnelt[3], U. Krewer[1]

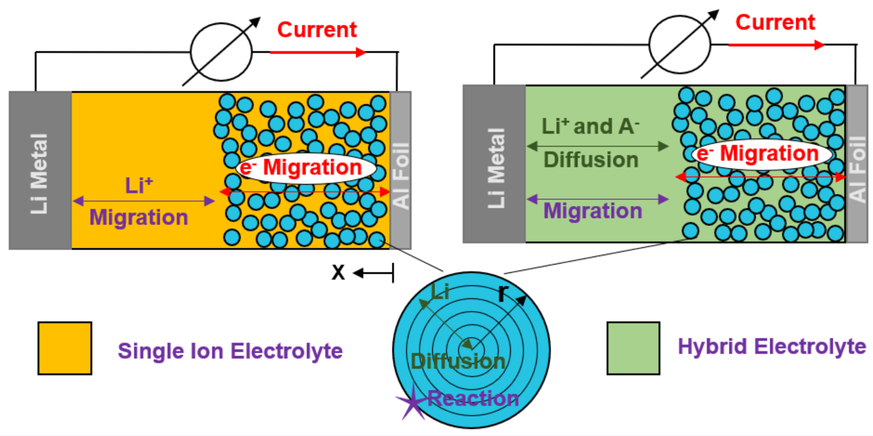
[1] Karlsruhe Institute of Technology, Institute for Applied Materials – Electrochemical Technologies, Adenauerring 20b, 76131 Karlsruhe, Germany

[2] TU Braunschweig, Institute of Energy and Process Systems Engineering, Langer Kamp 19b, 38106–Braunschweig, Germany

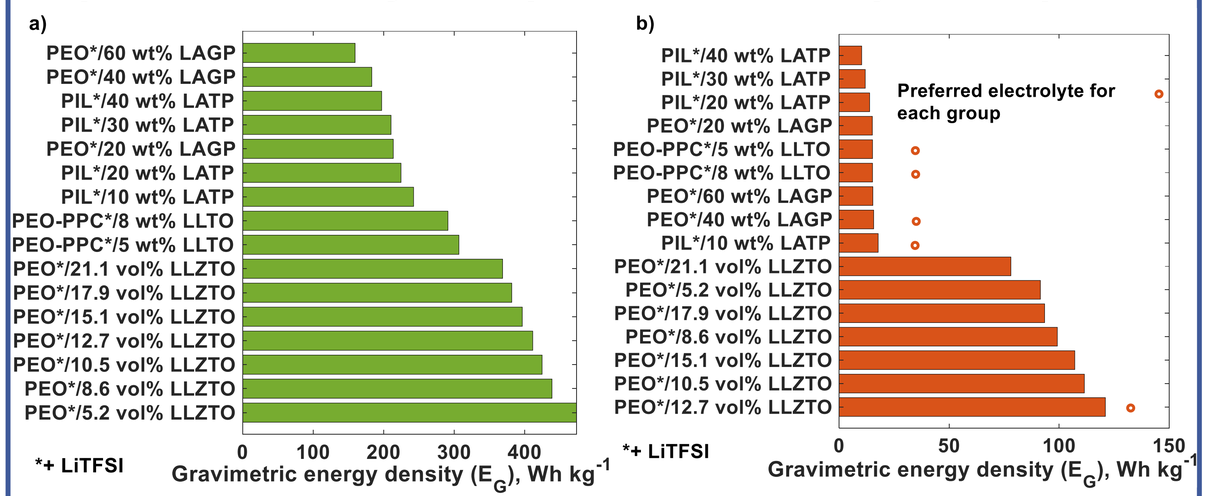
[3] Center for Low-Emission Transport –Electric Drive Technologies AIT Austrian Institute of Technology GmbH, Giefinggasse 2, 1210 Vienna, Austria

Motivation

- Development of all-solid-state batteries (ASSB) due to safety restrictions of liquid electrolytes [1].
- Utilising solid polymer composite electrolytes (SPCE) to improve contact between electrode and electrolyte [2].
- Applying P2D model for model-based evaluation of ASSB with hybrid electrolytes containing oxide and polymer.
- Identifying the best electrolyte with present technology and a potential attractive alternative electrolyte in future.



Impact of electrolyte on performance at a) 0.1C, b) 1C



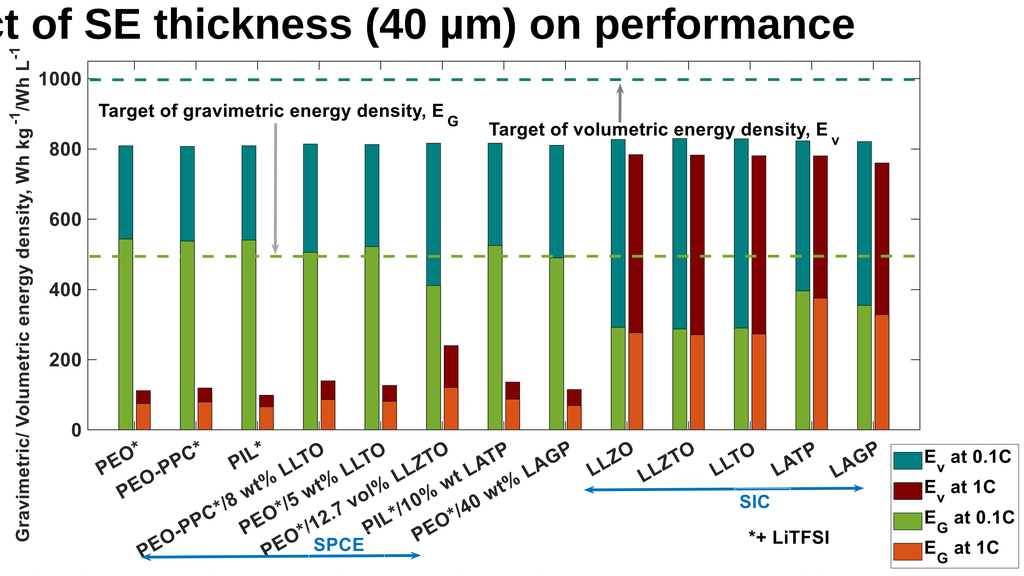
- ASSB based on 12.7 vol% of LLZTO is the best option based on present manufacturing constraints.

Optimisation results for ASSB with hybrid electrolytes

	δ_{cat}, µm	ε_s	E_G, Wh kg^{-1}	E_V Wh L^{-1}
Reference design, 0.1C	55	0.44	410.7	813
Optimal design for 0.1C	77	0.63	618	1251
Optimised cell for 0.1C, discharge at 1C	77	0.63	73.66	149.15
Reference design 1C	55	0.44	341.66	676.62
Optimal design for 1C	43	0.48	351.36	721.71
Optimised cell for 1C, discharge at 0.1C	43	0.48	395.44	812.26

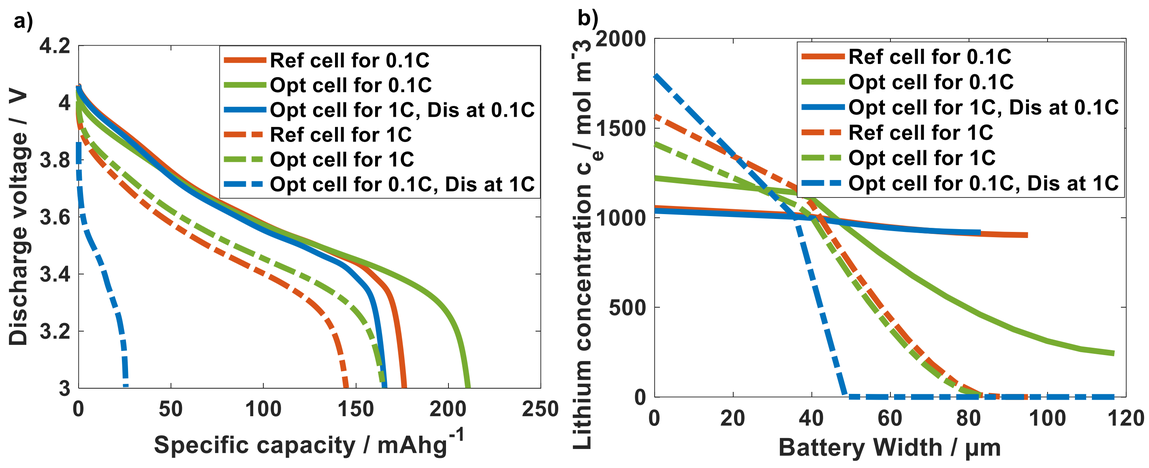
- Optimisation suggests a thicker cathode thickness (δ_{cat}) and higher volume fraction of active materials (ε_s) than reference cell.
- Optimal proposed design for a particular application doesn't perform well for all applications.

Effect of SE thickness (40 µm) on performance



- Single ion-conducting (SIC) electrolytes cannot achieve a higher gravimetric energy density than hybrid electrolytes.
- Hybrid electrolytes based on 10 wt% of LATP could be promising for future aircraft.

Insight into limitation within the batteries



- No evidence of ion starvation in cathode side for optimal cell at 0.1C
- The electrolyte overpotential at a higher current rate overcomes the benefit of increased theoretical capacity with increasing cathode thickness at optimal design point of 0.1C.

Conclusions

- Physics-based modelling in conjunction with an optimisation algorithm predicts optimal composition of ASSB for practically relevant C-rates.
- Optimal designs strongly depend on the concrete objective. Therefore, an aircraft power profile for better electrode design is necessary.
- Multilayer solid electrolyte, which combines advantages of two different electrolytes could allow to improve the gravimetric energy density of ASSB.

References

[1] J. Hoelzen et.al., Energies 11, 1 (2018). [2] G. Piana et.al., J. Energy Storage 26, 100947 (2019).

Acknowledgements

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