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## Understanding Electrolyte Infilling for Lithium Ion Batteries

*Tuesday, 1 June 2021 11:00 (15 minutes)*

Lithium ion batteries consist of three main porous components: anode, cathode and an electronically isolating membrane in between. This so-called separator prevents physical contact between the two electrodes while the pore space is filled with electrolyte to allow ionic transport. Therefore, the separator is considered to be a crucial part in battery safety.[1] Filling of the electrode and the separator with an electrolyte is a crucial and time-consuming step in the lithium ion battery manufacturing process and incomplete filling negatively impacts electrochemical performance, cycle life, and safety of cells.

Our research group has developed an approach to visualize and quantify a polyethylene (PE) separator with focused ion beam scanning electron microscopy (FIB-SEM).[2,3] The so-obtained 3D structure is used as a model system for typical polyolefin lithium ion battery separators, since it consists of a single solid phase with relatively uniform pore size and isotropic pore structure.

The 3D data set allows us to simulate the wetting of the separator membranes with liquid electrolyte. We perform quasi-static infilling simulations on the separator and show that during this imbibition-process up to 30% gas is entrapped in the separator. Using partial wetting theory, we show that the specific pore structure of the separator is responsible for this incomplete wetting.

A traditional parameter to characterize the performance of a separator is the effective transport coefficient (ratio between tortuosity and porosity). This value can be experimentally measured by electrical impedance spectroscopy (EIS).

Comparing the wetting simulations to these separator performance measurements, we demonstrate, that incomplete wetting can explain the discrepancy between theoretically predicted and experimentally measured transport coefficients. We also show that quasi-static wetting models overestimate the amount of residual gas in the membranes and that realistic wetting models have to consider both, the physio-chemical properties of the liquid electrolyte and the 3D structure of the separator pore space. Our work highlights the importance of pore structure in determining the amount of residual gas in a structure and provides insights into the pore structures, infilling conditions, and electrolyte formulations that are advantageous for battery technology.[4]

### Time Block Preference

Time Block A (09:00-12:00 CET)

### References

1. Zhang, S. S. A review on the separators of liquid electrolyte Li-ion batteries. *J. Power Sources* 164, 351–364 (2007).
2. Lagadec, M. F., Zahn, R. & Wood, V. Designing Polyolefin Separators to Minimize the Impact of Local Compressive Stresses on Lithium Ion Battery Performance. *J. Electrochem. Soc.* 165, A1829–A1836 (2018).
3. Lagadec, M. F., Müller, S., Zahn, R. & Wood, V. Topological and Network Analysis of Lithium Ion Battery Components: the Importance of Separator Pore Space Connectivity for Battery Operation.

4. Sauter, C., Zahn, R. & Wood, V. Understanding Electrolyte Infilling of Lithium Ion Batteries. J. Electrochem. Soc. 167, (2020).

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