

Building better batteries with insights from neutrons

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Since their introduction in 1991, lithium-ion batteries have become the popular choice for power sources in consumer electronics. Furthermore, as they have achieved a tremendous boost in their performance in the last decades, they are being increasingly employed in electrical vehicles and grid-scale energy storage systems as well. However, there is still room for improvement in terms of life expectancy, safety, cost, energy storage capabilities and interfacial stabilities. In this regard, understanding fundamental aging mechanisms that lead to capacity fade in Li-ion batteries becomes important to design batteries with improved components for performance enhancement.

With help of several examples, this presentation will reveal how different aging contributors such as loss of electrochemically active Li, active material degradation, and Li metal deposition can be detected using neutrons and conventional lab-based methods. For each of these cases, I will demonstrate how we optimized electrode design with feedback from obtained data and enhanced cell performance by positively affecting key parameters such as lifetime, charging rate, energy density, interfacial stability, and safety.

For example; using anodes containing mesocarbon microbeads instead of needle coke graphite we obtained faster charging capabilities and a longer lifetime [1]; by coating electrodes with polymers we achieved interfacial stability and obtained superior cycling performance [2]; by using Co-free cathodes and extending the operating voltage limits, we achieved both reductions in costs and increase in energy densities compared to conventional cathodes [3]; by incorporating silicon in anodes, we obtained increased energy densities compared to conventional anodes [4].

[1] N. Paul, J. Wandt, S. Seidlmayer, S. Schebesta, M. J. Mühlbauer, O. Dolotko, Hubert A. Gasteiger, R. Gilles, *Journal of Power Sources*, **85**, 345 (2017).

[2] Z. Huang, S. Choudhury, N. Paul, J. H. Thienenkamp, P. Lennartz, H. Gong, P. Müller-Buschbaum, G. Brunklaus, R. Gilles, Z. Bao, *Advanced Energy Materials*, **12**, 2103187 (2022).

[3] N. M. Jobst, N. Paul, P. Beran, M. Mancini, R. Gilles, M. Wohlfahrt-Mehrens, P. Axmann, *Journal of the American Chemical Society* **145**, 4450 (2023).

[4] N. Paul, J. Brumbarov, A. Paul, Y. Chen, J.-F. Moulin, P. Müller-Buschbaum, J. Kunze-Liebhäuser, R. Gilles, *Journal of Applied Crystallography*, **48**, 444 (2015).

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