Project CAESAR: Cell Chemistry Based on Silicon Anode and Nickel-Rich Cathode

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Project Overview

The new project CAESAR is a cooperation of the Technical University Munich (TUM) including the FRM II and several industrial partners (Fig. 1, 2). The aim of this project is the development of high-energy Li-ion batteries (LIB) with increased specific energy (Wh/kg) and energy density (Wh/l) accompanied by a decrease of the specific cost (€/Wh). To reach this, an appropriate combination of high-capacity materials is substantial, in this case Si anodes and Ni-rich layered oxide cathodes. Thereby, planned neutron studies at the FRM II will analyze LIBs with the aim to improve their performance. Main focus of this poster is the introduction of this just-started project in the context of the proposed neutron experiments. Besides that, first neutron depth profiling (NDP) results of differently lithiated Si anodes will be presented verifying a homogeneous depth distribution of Li throughout the anode, which is beneficial for their high cycling stability.

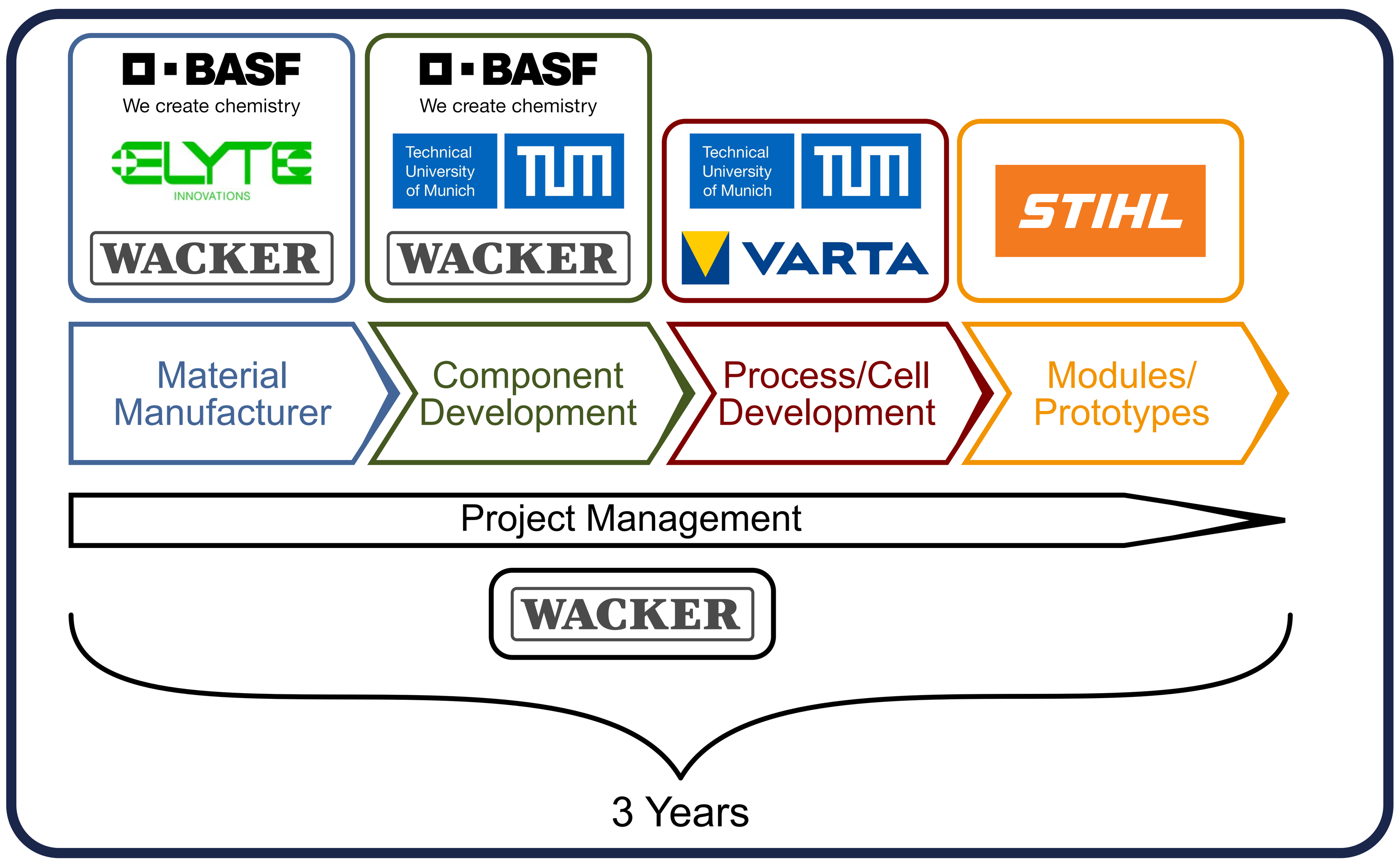


Fig. 1 | Project Organigram. Several partners cooperate to cover the whole value chain of lithium ion batteries.

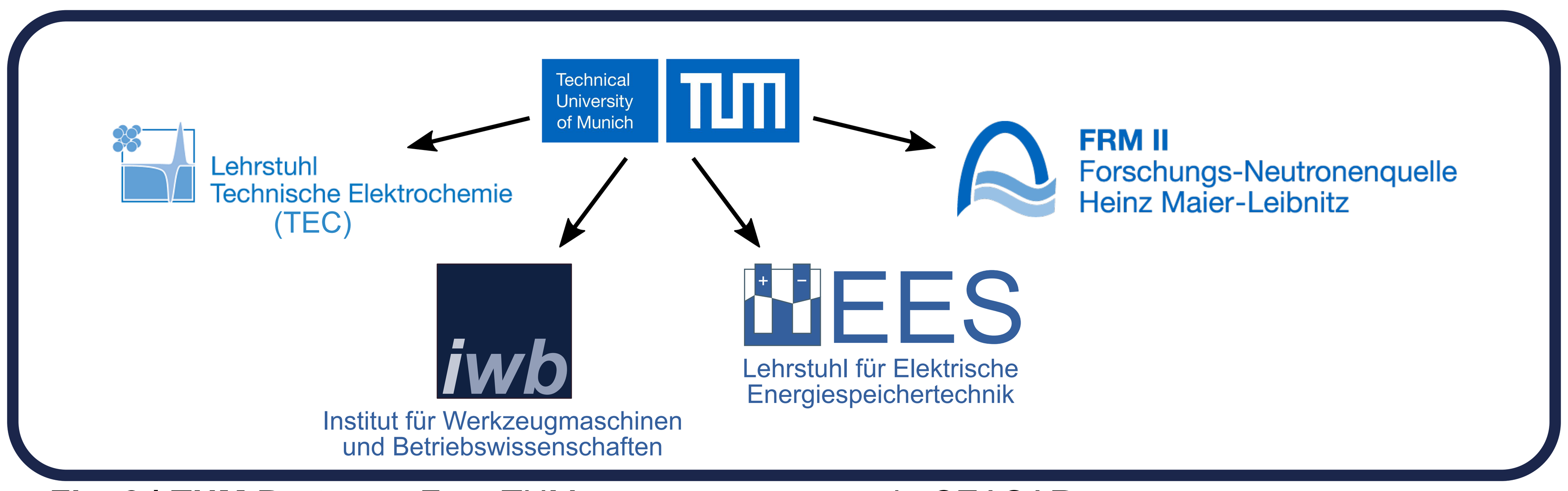
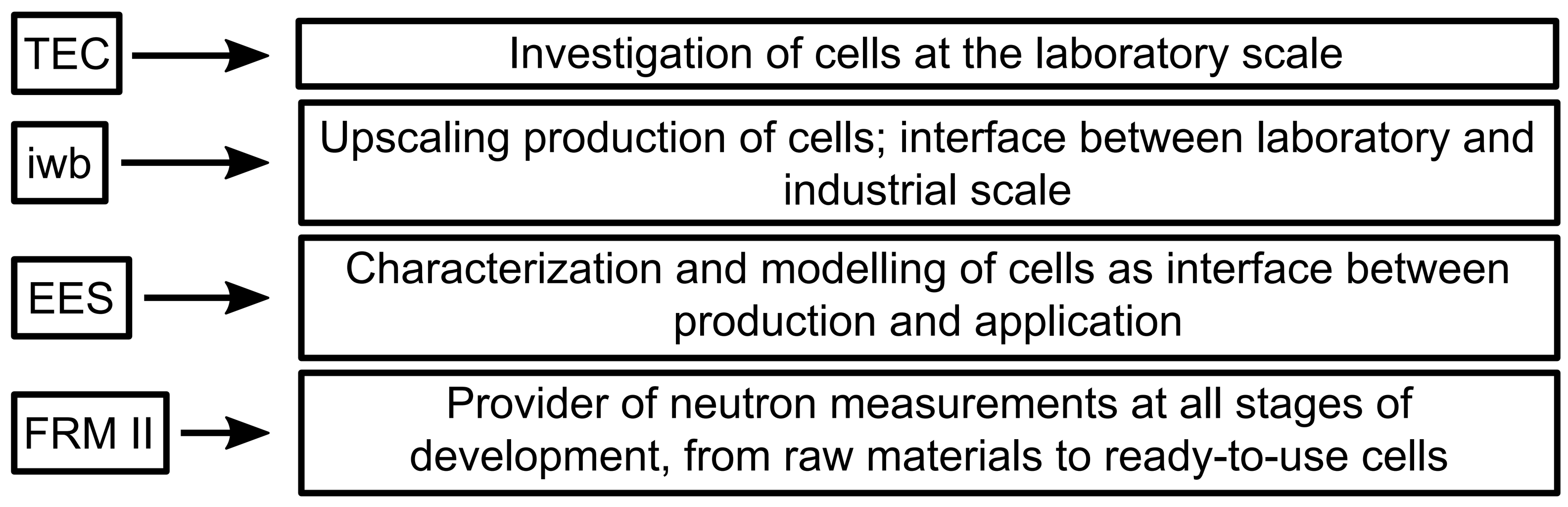
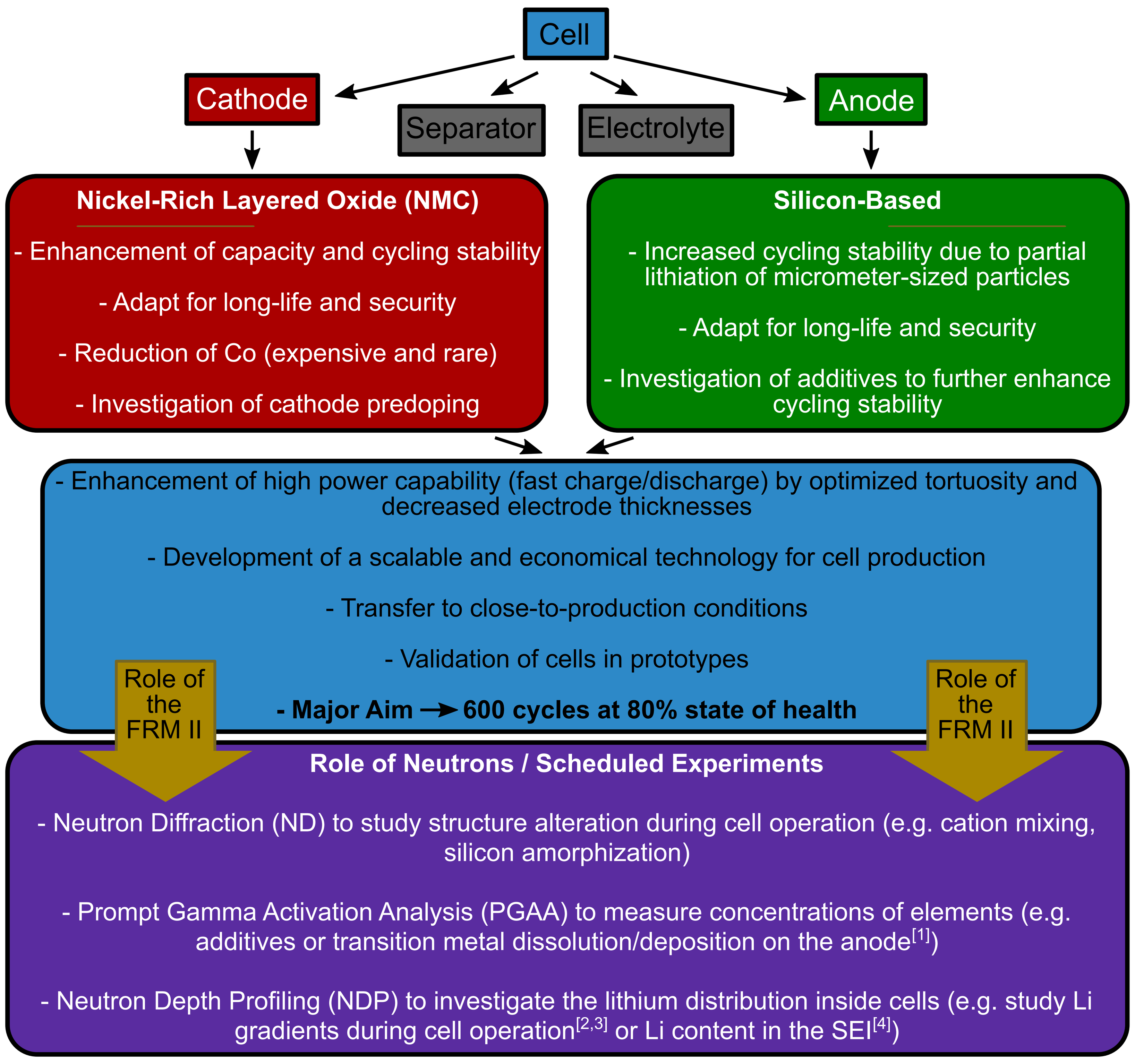


Fig. 2 | TUM Partners. Four TUM partners cooperate in CEASAR.



Aim and Scope of the Project / Role of the FRM II

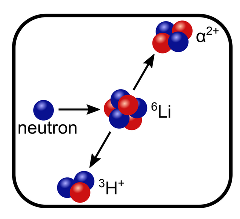


Why Silicon-Based Anodes?

Silicon anodes are promising candidates in order to increase the capacity of LIBs. The practical electrochemical capacity of Si amounting to 3579 mAhg^{-1} outrages the one of commonly used graphite of 372 mAhg^{-1}.[5] However, high volumetric changes of Si upon (de-)lithiation of ~300% lead to significant capacity reduction in Si-based anodes upon cycling.[6] To mitigate such unwanted effects, a novel strategy was introduced, whereby micrometer-sized Si particles are used as anode material and lithiation is only carried out partially to 30% (1080 mAhg^{-1}) of the maximum.[7] Furthermore, the electrolyte can be adapted to the high volume change of silicon. The electrolyte additive $LiNO_3$ improves the cycling stability of Si anodes.[8] This additive seems to lead to a more stable solid-electrolyte-interface (SEI) for Si particles. The mechanism is still unresolved and one focus of the CAESAR project.

Neutron Depth Profiling on Extracted Si-Based Anodes

- Nuclear Reaction: $^6Li + n \rightarrow {}^4He$ (2055 keV) + ^3H (2727 keV)
- Thickness measurement reveals swelling of Si due to lithiation (Fig. 3a)
- NDP reveals no gradients across the electrodes → homogeneous lithiation (Fig. 3b)
- Amount of Li in coating follows expected behavior



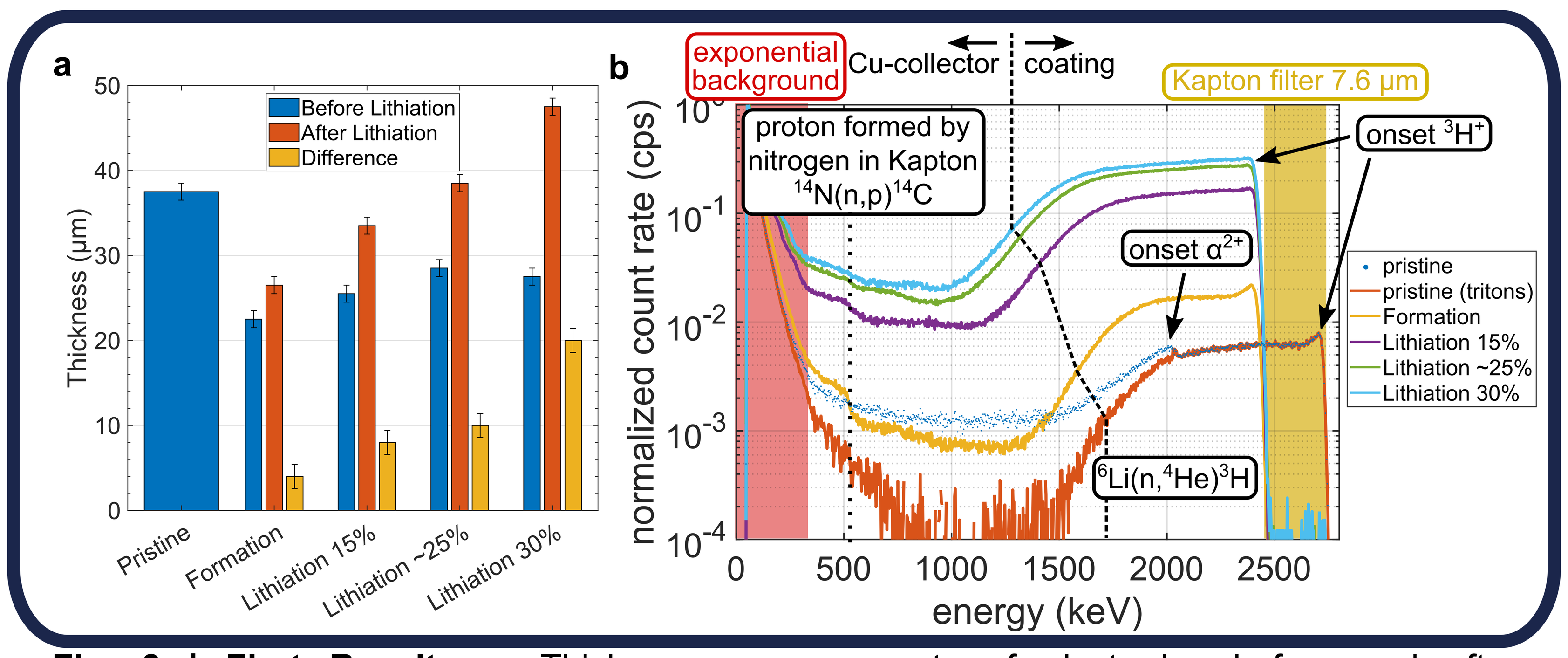


Fig. 3 | First Results. a Thickness measurements of electrodes before and after electrochemcial treatment. **b** NDP spectra of differently lithiated electrodes.

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