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Title: Stabilization of Lithium Metal Anodes with Porphyrin-based Electrolyte Additives

Acronym: SLAP

Consortium:

Danmarks Tekniske Universitet (DTU)

Helmholtz Institute, Ulm (HIU)

Karlsruhe Institute of Technology (KIT)

NanoScience Technology GmbH (NST)

ABSTRACT

The lithium ion battery (LIB) is currently the leading technology for rechargeable batteries. However, the LIB is reaching its performance limits. This challenge is being countered in research with the development of lithium metal batteries (LMBs), which feature a neat lithium metal anode instead of the lithium-carbon composite used in LIBs. The implementation of this technology would increase the anodic capacity more than tenfold. The key motivation here is that the use of a lithium metal anode will liberate volume within the battery to accommodate more cathode material. Furthermore, the freed volume in an LMB of the same size will render lithium iron phosphate (LFP), a more abundant, non-toxic, long-lasting cathode material, commercially viable for a much broader range of applications. However, the commercialization of LMBs is being hampered by the fact that the high-performance liquid electrolytes used in LIBs do not prevent the formation of Li-metal dendrites during repeated charge and discharge which leads to internal short circuits and potentially catastrophic battery failure. This funding application is concerned with the development of an effective solution to this problem, the addition of certain porphyrin-derivatives to the electrolyte in Li-metal cells, which increases the cycle life. The effect is presumably caused by incorporation of porphyrin derivatives into the solid-electrolyte-interface (SEI) layer. This effect might be unique to porphyrin derivatives, but may also occur with other porphyrin-derivatives, or phthalocyanines – in the following referred to as tetrapyrrole macrocycles (TPMs). The so modified SEI is evidently more effective at preventing the formation of dendrites in the long term. The successful implementation of this effect would be a game-changing breakthrough in the development of Li-based batteries with high capacities. The goal of the project is to showcase the viability of this additive-based approach to commercially realize LMBs with a liquid electrolyte in an industrially relevant environment. In order to achieve the goal it is planned to: experimentally investigate the formation process and the structure of the modified SEI formed by porphyrin derivatives as a basis for further optimization of the electrolyte; develop computational models of the underlying structure and the functional and mechanical properties of the modified SEI to predict pathways for further optimization; develop an optimized electrolyte composition on the

laboratory scale for use in an LMB with a commercially established cathode material; fabricate a full cell demonstrator device and validate its performance.