

Elektrocheminės Medžiagotyros Seminaras

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Importance of Advanced Interface Analytics for Rechargeable Batteries

Main challenges for long lasting batteries, especially when aiming for high energy density, stem from chemical and electrochemical interface stability, especially where active materials are in contact with electrolyte, due to the limited electrochemical stability window of current state-of-the-art electrolytes.

In this talk, firstly multifunctional electrolyte additives will be discussed with an emphasis on analytical matrix, where the importance of full cells for additive evaluation is shown. The Ni-rich layered oxides (Ni-rich NCMs) have a high practical specific capacity (180 mAh g^{-1} with the upper cutoff potential of 4.2 V vs. Li^+/Li), however, even higher capacity can be reached by Ni-rich NCM cathodes, if the voltage window is extended to potentials above 4.2 V. However, both limited anodic stability of the standard electrolytes above 4.2 V and instability of Ni-rich NCM cathode materials interface in a highly-charged state make high-voltage performance difficult to achieve. In this talk, two multifunctional additives [1,2] will be presented, mitigating the cycling stability issues of graphite||NCM851005 cell as a whole, as well as for preservation of graphite and Ni-rich layered oxide materials structures individually, even with high upper cutoff voltage up to 4.35 V (4.4 V vs Li^+/Li).

The second part is dedicated to well-studied additive fluoroethylene carbonate (FEC). Many reaction pathways have been proposed for FEC but there is currently no agreement on the exact type of chemical compounds, constituting the decomposition products, as well as on the mechanism of FEC decomposition. For this reason we conducted the systematic study, tracking morphological and chemical changes during electrochemical decomposition of FEC, and found that despite FEC often being referred as “film-forming” additive, in the first stage of its decomposition, spherical particles, mainly consisting of lithium fluoride, are formed.[3] And only later the carbonate-rich film covers the entire electrode, covering as well the LiF-rich spheres. This phenomenon has been overlooked by researchers earlier due to very simple reason (disclosed in the talk).

Literature:

- [1] H. Q. Pham, M. Mirolo, M. Tarik, M. El Kazzi, S. Trabesinger, *Energy Storage Materials*, 2020, **33**, 216-229.
- [2] H. Q. Pham, M. T. Nguyen, M. Tarik, M. El Kazzi, S. Trabesinger, *ChemSusChem* 2021, **14** (11), 2461-2474.
- [3] Y. Surace, D. Leanza, M. Mirolo, Ł. Kondracki, CAF Vaz, M. El Kazzi, P. Novák, S. Trabesinger, *Energy Storage Materials* 2022, **44**, 156-167.

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