

KFM 10: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 14:00–15:15

Location: H22

KFM 10.1 Tue 14:00 H22

Multiscale defective interfaces for realizing Na-CO₂ batteries with ultralong lifespan — ●CHANGFAN XU, TZUCHIN HUANG, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The cycling capability of Na-CO₂ batteries has been impeded by limitations in the kinetics of cathodic CO₂ reduction/evolution reaction (CO₂RR/CO₂ER) as well as the challenging process of depositing/stripping metallic Na during cycling.[1-3] Herein, a "two-in-one" electrode with multiscale defective FeCu interfaces (CP@FeCu) is presented, improving the kinetics of CO₂RR/CO₂ER and modulating sodium deposition behavior.[4] The enhancement of sodiophilicity and catalytic properties is attributed to multiscale defective FeCu interfaces, as revealed by experimental and theoretical investigations. The defect and valence oscillation effects originate in multiscale defective FeCu interfaces, effectively facilitating reactant adsorption and Na₂CO₃ decomposition during CO₂RR/CO₂ER processes, along with exceptional cycling stability of 2400 cycles (4800 h) at 5 μ A cm⁻². Meanwhile, the CP@FeCu with high sodium affinity creates a uniform electric field and strong Na adsorption, promoting favorable nucleation sites for dendrite-resistant and durable anodes. This work provides scientific insights into the design of "two-in-one" electrodes, which are crucial for addressing challenges in sodium anodes and CO₂ cathodes. [1] Small 2023, 2206445 [2] Adv. Funct. Mater. 2023, 2300926 [3] Energy Environ. Mater. 2024, 7, e12626 [4] Adv. Mater. 2024, 2409533

KFM 10.2 Tue 14:15 H22

Electro-chemo-mechanical behavior of a layered cathode material upon cycling — ●ROBERT LÖSER¹, YUG JOSHI², ROHAM TALEBI¹, and GUIDO SCHMITZ¹ — ¹University of Stuttgart, Stuttgart, Germany — ²Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

The mechanical properties of lithium-ion cathode materials play a critical role in determining battery performance such as cycle life, durability, and safety, especially when the battery is under external pressure which is typical for all-solid-state batteries. This research investigates LiCoO₂ (LCO), a prevalent hexagonal layer-structured cathode material, and explores its mechanical responses during de-/lithiation using sputter-deposited thin films and nanoindentation. The values of the experimental Young's modulus in pure (101) and (003) lattice orientations are quantified to 337.1 \pm 8.7 GPa and 267.9 \pm 7.2 GPa, respectively, in the fully lithiated state. Furthermore, a substantial texture-dependent decrease in Young's modulus upon lithium deintercalation is demonstrated, probably due to modification of the bonding interactions between the cobalt oxide layers. Delithiation also elevates the relative contribution of plastic deformation, indicating that dislocation glide becomes easier in deintercalated states. By extensive cycling, the Young's modulus in higher lithiated charge-states decreases considerably which is most-likely due to irreversibility of phase transitions. The work provides valuable insight on the dynamic changes of the mechanical properties during electrochemical cycling of LiCoO₂, which paves the way for all other layered cathode materials.

KFM 10.3 Tue 14:30 H22

MnTiO₃ as a Carbon-Free Cathode for Rechargeable Li-Oxygen Batteries — DOAA AHMED^{1,2}, WERNFRIED MAYR-SCHMÖLZER¹, MUSTAFA ÇELİK^{3,4}, ABDULKADIR KIZILASLAN^{3,4}, and ●GREGOR VONBUN-FELDBAUER^{1,2} — ¹Institute of Advanced Ceramics, TU Hamburg, Germany — ²Institute of Soft Matter Modeling, TU Hamburg, Germany — ³Research, Development and Application Center (SARGEM), Sakarya University, Turkey — ⁴Department of Metallurgical and Materials Engineering, Engineering Faculty, Sakarya University, Turkey

Lithium-oxygen batteries (LOB) are promising energy storage systems due to their high theoretical energy density. However, their main challenges are the sluggish kinetics of oxygen reduction and evolu-

tion reactions (ORR/OER) and high charge overpotentials. To overcome these challenges, the development of a suitable catalyst is crucial. Here, MnTiO₃ was investigated as a carbon-free cathode catalyst using density functional theory (DFT) calculations and experimental approaches. DFT calculations revealed the coexistence of Mn and Ti energy levels near the Fermi level of MnTiO₃, which facilitates ORR/OER. This feature endows MnTiO₃ with a bifunctional role in promoting battery performance. Our DFT-based investigation further elucidates the surface stability and catalytic properties of MnTiO₃. In addition, experiments confirm that the electrochemical reactions on MnTiO₃ follow a two-electron pathway. LOBs with MnTiO₃ exhibit a total overpotential of 1.18 V and 1.55 V from DFT and electrochemical measurements, respectively, and current densities up to 1 A/g.

KFM 10.4 Tue 14:45 H22

Modeling and optical characterization of Lithium deposition on Copper current collectors — ●LEN KIMMS¹, TJARK INGBER², DIDDO DIDDENS^{1,2}, and ANDREAS HEUER¹ — ¹Institut für physikalische Chemie, Universität Münster — ²Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH

In this contribution, we will present modeling results of the initial deposition of lithium metal on a copper current collector combined with experimental insights. Zero-excess lithium-metal batteries (ZELMBs) may offer higher energy densities, better safety, and reduced cost by reducing the amount of lithium employed in the cell. Instead of an excess of lithium as electrode, the anode is formed in situ during charging. When charging the battery, lithium is plated on the current collector directly. However, the lifespan of ZELMBs in practical applications is still limited by irreversible loss of active lithium. The loss is induced by the high reactivity of lithium which causes parasitic side reactions and dendrite growth during charging cycles. To uncover the mechanisms at play, the initial deposition of lithium metal has been experimentally investigated by plating varying amounts on a copper surface with different current densities. The deposits have been characterized by scanning electron microscopy (SEM) and laser scanning microscopy (LSM) in an automated way. Numerical simulations of a simple geometric model were employed to uncover the relevant mechanisms which govern the growth over different stages. Combining the experimental and numerical results, an effective description of the deposition has been found.

KFM 10.5 Tue 15:00 H22

Preparation of Prussian blue analogue materials and their application to potassium-ion batteries — ●PING HONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Prussian blue (PB) and its analogs (PBAs), with their unique open framework structure and chemical stability, have emerged as promising cathode materials for potassium-ion batteries (PIBs). PB and PBAs feature three-dimensional channels, facilitating rapid potassium-ion intercalation and de-intercalation, thus delivering excellent rate performance. Furthermore, its low-cost synthesis and environmentally friendly properties provide a strong foundation for potential commercial applications. Despite these advantages, the practical application of PBAs is hindered by challenges such as their high solubility in electrolytes and limited cycle stability and life. To overcome these limitations, we optimized synthesis techniques (by simple adjustment of the co-precipitation method) and structural design, leading to significant improvements in material performance. In addition, a series of adjustments were made to the binder, electrolyte, and voltage range used in the batteries. The improved PBA cathode exhibited remarkable cycling stability, showing almost no capacity decay after 500 cycles at a current density of 100 mA/g within the voltage range of 2.0-4.0 V. It maintained excellent cycling performance even under high current conditions, providing strong support for the advancement of high-performance PIBs.