CPP 4: Energy Storage Materials and Devices I

Time: Monday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 4.1 Mon 9:30 ZEU/0255

Exploration of Cathode Materials for Li-S Batteries — •Yan Lu — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Recently, a lot of efforts have been devoted into lithium-sulfur (Li-S) battery system due to its high theoretical capacity (1675 mAh g-1) and low cost, which could be a competitive candidate for the next-generation batteries in the future. However, it suffers from a poor cycling stability during charging-discharging, which is blamed to the "shuttle effects" of lithium polysulfides. Fundamental understanding of the formation and dissolution processes of both solid phases, S8 and Li2S, is necessary for the development of advanced cathode materials (both organosulfur and metal compound-based sulfur host) with improved electrochemical performance. Synchrotron-based operando high-resolution X-ray imaging has been successfully used for the detailed morphology study of sulfur particles during cycling of the battery cells. Using colloidal route, complex hybrid carbon nanostructures have been synthesized using colloidal polymeric particle as soft template, which have been applied as cathode materials for Li-S batteries.

CPP 4.2 Mon 10:00 ZEU/0255

Temperature-dependent Crystal Structure of Dimethyl Carbonate — •Lea Westphal[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

The performance and safety/stability of Li-ion batteries (LIBs) can be enhanced by optimizing the charge-storing electrode materials and/or the charge-mediating liquid electrolytes. In LIB research, the major focus has been on the electrode subsystem, while liquid electrolytes are studied much less. Upon cooling of LIBs to investigate their performance at low temperatures, a series of Bragg reflections has been observed, which was assigned to the freezing of liquid electrolyte. Further measurements reveal the development of long-range order in the model electrolyte mixture LP30. To better understand this emerging order, it is essential to investigate the system's individual components, especially under conditions near room temperature relevant to in situ sub-ambient LIB studies.

This contribution outlines our efforts to crystallize Dimethyl Carbonate with minimized preferred orientation, in order to study the unit cell across the entire solid temperature range using neutron- and synchrotron-based powder diffraction. The datasets are complemented by synchrotron single-crystal diffraction experiments. Additionally, the liquid state is investigated by Total Scattering and Pair Distribution Function analysis.

CPP 4.3 Mon 10:15 ZEU/0255

Electron Energy Loss Spectroscopy for oxidation state analysis on ammonia synthesis catalysts — •Daniela Ramermann, Michael Poschmann, Elisabeth H. Wolf, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim (Ruhr)

Electron energy loss spectroscopy (EELS) is a powerful technique, not only for the determination of elemental compositions, but also for the investigation of chemical bonding and oxidation states. For the analysis of EELS data, the use of cross-section models is quite common, but the use of reference spectra improves the quantification results. In addition, it allows for the fitting of the edge shapes to investigate oxidation states with the spatial resolution of the electron microscope.

Because the available databases for EELS references [1] are not exhaustive, reference materials are obtained from acquired commercial materials of well-known and defined properties. It is crucial to thoroughly characterize these materials before measuring the reference spectra, as the materials may have local impurities or differ from the desired oxidation state. For the Fe-based catalyst system some reference materials are of mixed oxidation state, presenting an additional challenge.

We show the process of acquiring suitable EELS references for materials used in catalysis and the application of mapping the oxidation state and phase composition on a Fe based ammonia synthesis catalyst.

[1] https://eelsdb.eu, https://eels.info/atlas

CPP 4.4 Mon 10:30 ZEU/0255

Investigating the Conversion Reaction of the Cathode Active Material FeS_2 in Solid-State Batteries via Transmission Electron Microscopy — •Franziska Hüppe[1], Matilde Pavan[2], Shamail Ahmed[1], Jürgen Belz[1], Jürgen Janek[2], and Kerstin Volz[1] — [1]Philipps-Universität Marburg, Department of Physics and mar.quest, Hans-Meerwein-Straße, 35043, Marburg, Germany — [2]Justus-Liebig-Universität Gießen, Institute of Physical Chemistry and Center for Materials Research, Heinrich-Buff-Ring, 35392, Gießen, Germany

Solid-state batteries are particularly promising for high-energy storage, as they potentially allow for the use of electrode materials with higher specific capacities. In the case of FeS_2 as cathode active material, also the cost effectiveness and the environmental impact would be drastically enhanced. However, FeS_2 is a conversion-type material that undergoes continuous compositional and structural changes during cycling that is not yet fully understood at the micro- and nanoscale.

Scanning transmission electron microscopy (STEM) offers structural insights at high resolution and is combinable with deepening investigation methods like energy dispersive X-ray spectroscopy (EDX) and electron energy loss spectroscopy (EELS) to identify the different compounds forming during different depth of discharge (lithiation).

The pristine, uncycled cathode sheet contains FeS_2 particles with cubic structure. With increasing depth of discharge, the particles react from the outside in, forming core-shell structures. The multimodal STEM analysis will be discussed in detail during the presentation.

CPP 4.5 Mon 10:45 ZEU/0255

Dual-cation pre-intercalated hydrated vanadium oxide for ultralong cycling stability in aqueous zinc-ion batteries — •Yan Ran, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

In this work, hydrated vanadium oxide with pre-intercalated K and Mn ions (K0.07Mn0.13V2O5*1.47H2O) was synthesized via a one-step hydrothermal method, demonstrating an excellent specific capacity of 524.7 mA h g-1 at 0.1 A g-1, and outstanding stability with 82.47% capacity retention after 20,000 cycles at 5 A g-1. The co-intercalation of dual cations increases the interlayer spacing while stabilizing the material structure, expanding the ion transport channels, and improving both the specific capacity and long-cycle stability. Moreover, the Zn2+/H+ co-intercalation mechanism was confirmed by ex-situ characterization. This work will provide insights for the development of competitive cathodes in high-performance aqueous batteries.

CPP 4.6 Mon 11:00 ZEU/0255

Unveiling the Interfacial Behavior of Lithium Batteries by Operando X-ray Scattering — •Yuxin Liang[1], Fabian Apfelbeck[1], Kun Sun[1], Yingying Yan[1], Lyuyang Cheng[1], Guangjiu Pan[1], Tianle Zheng[1], Yajun Cheng[2], Anton Davydok[3], Christina Krywka[3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]College of Renewable Energy, Hohai University, Changzhou, China — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Poly(ethylene oxide) based solid composite electrolytes suffer from poor conductivity and lithium dendrite growth, especially toward the metallic lithium metal anode. In our recent work, we focus on the fabrication and comprehensive characterization of performance-enhanced PEO-based composite electrolytes for lithium batteries. Advanced nano-focus X-ray scattering techniques were used to investigate the interfacial behavior within the lithium metal battery, as well as its failure mechanisms. With the modification of plasticizer, the electrolyte exhibit good electrochemical performance and interfacial compatibility. However, the reference electrolyte exhibit early dendrite formation from the lithium surface into the electrolyte, leading to persistent structures that degrade performance. The results highlight the potential of these fabrication and analysis methods, demonstrating their application in advancing lithium battery technologies and contributing to the development of cutting-edge characterization techniques.