CPP 40: Energy Storage and Batteries II

Time: Friday 9:30–11:15 Location: H34

CPP 40.1 Fri 9:30 H34

Nanoscale Agglomeration Mechanisms of BF-DPB:BPyMPM Donor-Acceptor Systems for Organic Optoelectronic Devices — •Milena Merkel[1], Philipp Wiesener[1], Robert Schmidt[1], Rishi Shivhare[2,3], Rudolf Bratschitsch[1], Saeed Amirjalayer[4], Koen Vandewal[2,3], and Harry Mönig[1] — [1]Physikalisches Institut, Münster University, Münster, Germany — [2]Institute for Materials Research (imo-imomec), Hasselt University, Hasselt, Belgium — [3]imec, imo-imomec, Diepenbeek, Belgium — [4]Interdisciplinary Center for Scientific Computing, Heidelberg University, Heidelberg, Germany

The molecular order of photo-active molecules of organic optoelectronic devices has major impact on their performance. However, it is usually investigated only by indirect measurements or simulations. Here we use low-temperature scanning probe microscopy to image the molecular assembly and interfaces of the donor and acceptor molecules BF-DPB and BPyMPM with submolecular resolution. We illustrate the crucial effect of the substrate and the position of the nitrogen atoms in the BPyMPM molecules on the formation of intermolecular C-H..N hydrogen bonds, metal coordination bonds and corresponding self-assemblies. Using scanning tunneling spectroscopy, we are able to correlate the increasing disorder at the BF-DPB:BPyMPM interface with an increase in the HOMO-LUMO gap of BF-DPB. Photoluminescence measurements on BF-DPB indicate a significant increase in intersystem crossing due to molecule-substrate interactions. Our results provide new insights for a tailored design of active molecules and contact layers for organic optoelectronic devices.

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Multi-layered electrodes for flexible solid-state super capacitors with polymer-based gel electrolyte — •Reyhaneh Bahramian[1,2,3] and Yaser Abdi[3] — [1]Department of Cognitive Sciences, Faculty of Psychology and Education, University of Tehran, Tehran, Iran — [2]Condensed Matter National Laboratory, Institute for Research in Fundamental Sciences, Tehran 19395-5531, Iran — [3]Nanophysics Research Laboratory, Department of Physics, University of Tehran, Tehran 14395-547, Iran

Flexible solid-state supercapacitors are gaining popularity due to their advantages, including flexibility, lightweight design, high power density, rapid charge and discharge rates, broad operating temperature ranges, long cycle life, safety, and ease of fabrication. The use of gel polymer electrolytes enhances ionic conductivity while addressing safety concerns associated with liquid electrolytes.

This research focuses on developing nanocomposite electrodes using Ag-decorated zinc oxide, synthesized through a chemical deposition method on carbon paper, and ferrite applied via a drop-casting technique. The goal is to create electrodes that can operate across a wide voltage range in a non-aqueous electrolyte.

Advanced characterization techniques, such as atomic force microscopy, X-ray diffraction, field emission scanning electron microscopy, and Raman spectroscopy, are employed to analyze the structural properties of the electrodes. The findings reveal an effective specific capacitance of approximately 70 milliFarads per square centimeter.

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Dual-cation pre-intercalated hydrated vanadium oxide achieves 20,000 cycles in aqueous zinc-ion batteries — •Yan Ran and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Aqueous zinc-ion batteries (AZIBs) have broad application prospects in energy storage due to their low cost and high safety. However, cathode materials still face challenges such as low specific capacity and decreased long-cycle performance. 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 40.4 Fri 10:15 H34

Temperature-resolved Crystal Structure of Ethylene Carbonate — •Lea Westphal[1,2], Vladislav Kochetov[2], Volodymyr Baran[3], Maxim Avdeev[4,5], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany — [3]DESY, 22607 Hamburg, Germany — [4]ANSTO, NSW 2234, Sydney, Australia — [5]School of Chemistry, University of Sydney, NSW 2006, Sydney, Australia

Lithium-ion batteries (LIBs) have been a dominant power source for portable electronics for over three decades and are of interest for applications in electric vehicles and large-scale energy storage systems. Despite significant advancements in LIB design, the main solvents used in the liquid electrolytes, responsible for the charge transfer between the electrodes, have largely remained the same. A key class of these solvents are linear and cyclic carbonates, which, when two or more solvents are combined with lithium salts and additives, exhibit favorable physical/chemical properties. Ethylene carbonate (EC) is a common solvent in commercial batteries due to its high dielectric constant and its ability to form the protective solid-electrolyte interphase (SEI) layer. However, it has to be mixed with other solvents because of its high melting point. Following the determination of EC's crystal structure from single crystals, this study presents temperature dependent Neutron and Synchrotron Powder Diffraction data, studying the sample from 3 K up to its melting point and investigations by Synchrotron Total Scattering and Pair Distribution Function analysis.

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Polymer-nano-tufts: A hairy story of limited conductivity — •Martin Tress, Alaa Yussef Hassan, Nico Junkers, and Wing Kit Or — Peter-Debye-Institute for Soft Matter Research, Leipzig University, Leipzig, Germany

Here we present an approach to study conductivity in small polymer aggregates of as few as ten chains using dielectric spectroscopy [Macromol Chem Phys, 224 (2023) 2200452]. For that, a nano-structured electrode arrangement is combined with several physico-chemical surface modifications to deposit a regular pattern of gold nanoparticles onto which end-functionalized polymer chains are grafted to create tuft-like ensembles of individualized chain aggregates. For polyethylene, pronounced changes in conductivity are observed in tufts compared to bulk with details indicating an alteration of the type of charge transport. This might signal a switch from fast inter-chain ion hopping, dominating in bulk, to slower intra-chain ion hopping in the tufts attributed to the chain configurations and orientation forced by the grafting. Consequently, this could be a more general phenomenon of polymer-solid interfaces that may explain significantly increased electrode polarization and interfacial resistance in ion-conducting polymers, potentially diminishing their performance. Hence, the hypothesis, that bottle-brush architectures could reduce these unwanted effects, was developed. Supported by preliminary results, this might be a step to improve polymeric electrolytes for various fields ranging from solid-state electrolyte batteries to ion-conducting fuel cell membranes.

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Interpretation of the Impedance Signal of Composite Materials using a 3D Electrical Network Model — •Felix Schug[1,2], Sascha Kremer[2,3], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, 35392 Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, 35392 Giessen, Germany

All solid-state batteries (aSSBs) are promising candidates for next-generation energy storage systems, offering high energy and power densities as well as improved device safety compared to the established lithium-ion batteries. Electrochemical impedance spectroscopy (EIS) is one of the key methods to determine charge transport characteristics of the material components in an aSSB. Many of these components are composed of multiple phases, with various transport processes affecting the impedance response signal. Furthermore, the microstructure of the material manifests as a signal within the impedance spectrum. The interpretation of an impedance spectrum is therefore not straightforward, as many signals overlap or are indistinguishable from each other. We therefore employ a microstructure-resolved 3D electrical network to modulate charge transport on microscopic length scales. This approach reveals how microstructure affects the impedance response, as well as the potential and current distributions within a system. It is used to investigate the impedance of composite materials and to develop guidelines for its interpretation.

CPP 40.7 Fri 11:00 H34

Measuring Local Electrochemical Properties with Scanning Probe Microscopy — •Alexander Klasen and Andrea Cerreta — Park Systems Europe GmbH, Mannheim, Germany

Electrochemical (EC) applications, ranging from novel energy storage systems to advanced catalysts, are defined on an ever-decreasing length scale. Investigating these systems requires to map key functional features with sufficient resolution, such as the local structure, electronic properties and electrochemical response. Scanning probe microscopy-based techniques are well established to investigate surface parameters using the physical interaction with a nanometer-sized probe allows studying properties such as the topography, work function, or adhesion at high resolution. One such technique, Scanning Electrochemical Cell microscopy (SECCM), was first introduced by E. Daviddi, P.R. Unwin, et al. and uses a pipette-based SPM approach to probe local EC features. When brought in close proximity to the sample, the electrolyte-filled pipette pipette creates a small electrolyte meniscus between the pipette aperture and the surface of interest . This confined volume of solution constitutes a small electrochemical cell that allows for local measurements of electrochemical characteristics. In this talk, we discuss the basics of SECCM, present recent examples from literature, discuss the limitations of the technique and outline potential pathways to overcome those.