International Graduate School
BACCARA

Supervisor Guide
Core Interests:

- Electrochemistry and electrocatalysis
- Nonlinear optical laser spectroscopy at interfaces
- Molecular self-assembly at interfaces
- Molecular control of interface-rich materials
- Colloids, foams and nanoparticles


Selected Publications:

Core Interests:
- Development of OLEDs
- Development of organic solar cells
- N-heterocyclic carbenes
- Metal-bridged DNA
- 2d materials
- Light-controlled materials

Homepage: https://www.uni-muenster.de/Physik.FT/en/Forschung/agdoltsinis/index.html

Selected Publications:
Prof. Dr. Melanie Esselen

Core Interests:

The current research of Prof. Dr. M. Esselen focuses genotoxic and mutagenic effects and combinatory toxicity of food constituents and environmental contaminants. Further, the group is interested in cell culture studies to investigate the impact of compound classes on key elements of cellular signaling cascades such as Nrf-2 pathway, apoptosis or DNA-topology in cells and humans. The third focus include analysis aspects e.g. toxicokinetic in cell culture systems and in humans.

Homepage: https://www.uni-muenster.de/Chemie.lc/en/forschung/esselen/prof.dr.esselen.html

Selected Publications:


Core Interests:
• Organic Synthesis
• N-Heterocyclic Carbenes
• Organocatalysis
• Asymmetric Catalysis
• C-H Activation
• MOFs
• Heterogeneous Catalysis
• Photoredox-Catalysis
• Smart Screening Technologies
• Electrolytes/Batteries

Homepage: https://www.uni-muenster.de/Chemie.oc/glorius/glorius.html

Selected Publications:
Core Interests:

- Polymer synthesis
- Functional polymer nanostructures
- Multicompartiment microparticles
- Polymer templates for catalysis

Homepage: https://www.uni-muenster.de/Chemie.pc/en/forschung/groeschel/prof.dr.groeschel.html

Selected Publications:

Core Interests:

- In situ and in operando NMR studies of Li-ion batteries
- NMR characterization of structure and dynamics in solid-state electrolytes
- Ion dynamics in solid-state electrolytes
- Soft matter and polymer materials
- Development of solid-state NMR methods

Homepage: https://www.uni-muenster.de/Chemie.pc/en/forschung/hansen/hansen.html

Selected Publications:


**Core Interests:**
The field of activity comprises both basic and applied research in food and bioanalytics using hyphenated mass spectrometric techniques and high-resolution mass spectrometry:

- Lipids
- Double bond position determination in lipids
- Software development for lipid identification
- Biosurfactants
- Analytics of Metabolites
- Dielectric barrier discharge ionization

**Homepage:** [https://www.uni-muenster.de/Chemie.ac/en/hayen/hayenresearchgroup/professorhayen/index.html](https://www.uni-muenster.de/Chemie.ac/en/hayen/hayenresearchgroup/professorhayen/index.html)

**Selected Publications:**

- J. Henschel, H. Hayen, MethodsX 7 (2020) 101134. *Application of large volume injection for sensitive LC-MS/MS analysis of seven artificial sweeteners in surface waters.*


Core Interests:

- Multiscale simulations for a variety of different applications:
  - Battery-inspired systems (e.g. liquid and polymeric electrolytes, electrolyte/electrode interfaces)
  - Soft matter systems (e.g.. Membranes/Biomolecules, Structure formation)
  - Disordered systems
- Conceptual developments (e.g., incorporation of chemical rates into molecular dynamics simulations)
- Data-driven analysis (e.g., machine learning for the analysis of experimental HTS electrolyte data)

Homepage: https://www.uni-muenster.de/Chemie.pc/en/forschung/heuer/prof.dr.heuer.html

Selected Publications:

Core Interests:

HPLC-MS/MS analysis, metabolism, toxicity and bioavailability of food contaminants and environmental chemicals as well as human exposure.

Homepage: https://www.uni-muenster.de/Chemie.lc/en/forschung/humpf/prof.dr.humpf.html

Selected Publications:

Core Interests:

• Autodisplay of proteins for drug discovery and biotechnology applications
• Bioeconomy
• Enzymatic conversion of plant biomass into basic chemicals
• Biotechnology-based sustainable chemistry
• Enzyme recycling

Homepage: https://www.uni-muenster.de/Chemie.pz/forschen/ag/jose/index.html

Selected Publications:


Core Interests:

- Electrochemistry-Mass Spectrometry
- Hyphenated techniques
- Nanoparticles
- Speciation Analysis
- Applied Atomic Spectroscopy

Homepage: https://www.uni-muenster.de/Chemie.ac/en/karst/karst.html

Selected Publications:


Core Interests:

- Technology and Innovation Management
- Sustainability and Recycling
- Battery Cost Modelling
- Life Cycle Assessment (LCA)

Homepage: https://www.uni-muenster.de/Chemie.bm/institut/leker.html

Selected Publications:

Core Interests:

- Electronic-Structure Theory: Method Development and Software Implementation
- Energy and Electron Transfer in Molecular Aggregates
- Quantum Chemical Characterization of Molecular Electric and Magnetic Properties
- Theoretical Spectroscopy
- Computational Analysis of Reaction Mechanisms in Molecular and On-Surface Chemistry

Homepage: [https://www.uni-muenster.de/Chemie.oc/neugebauer/neugebauer.html](https://www.uni-muenster.de/Chemie.oc/neugebauer/neugebauer.html)

Selected Publications:


Core Interests:

- Self-Assembly
- Supramolecular Materials
- Nanoparticles and Nanocontainers
- Surface Functionalization

Homepage: https://www.uni-muenster.de/Chemie.oc/ravoo/ravoo.html

Selected Publications:

Core Interests:

• Biosynthesis of microbial polysaccharides
• Tailoring of microbial polysaccharides for future applications
• Optimization of the fermentative production of microbial polysaccharides
• Genetic strain engineering

Homepage: https://www.uni-muenster.de/Biologie.IMMB.Schmid/en/index.html

Selected Publications:

• Rütering M, Cress BF, Schilling M, Rühmann B, Koffas MAG, Sieber V, Schmid J, Tailor-made exopolysaccharides - CRISPR-Cas9 mediated genome editing in Paenibacillus polymyxa, Synthetic Biology (2017) 2 (1)
Core Interests:

• NMR studies of molecular transport by Pulsed Field Gradient methods
• Ion transport mechanisms in battery electrolytes
• Liquid, polymeric and gel electrolytes
• Functional polymer materials from polyelectrolytes
• Porous Materials and Colloidal Carriers

Homepage: https://www.uni-muenster.de/Chemie.pc/en/forschung/schoenhoff/prof.dr.schoenhoff.html

Selected Publications:

• Ackermann, F.; Schönhoff, M.; Chelating Additives Reversing the Lithium Migration Direction in Ionic Liquid Electrolytes, J. Phys. Chem. C 2021, 125, 266-274.


Core Interests:

- Radical Chemistry in Organic Synthesis – Method Development
- Radicals and Catalysis
- Systems Chemistry – Organic Chemistry at Interfaces and in Hybrid Materials

Homepage: https://www.uni-muenster.de/Chemie.oc/studer/studer.html

Selected Publications:


Jun.-Prof. Dr. Stephan von Delft

Core Interests:

• Strategy and Entrepreneurship
• Sustainability and recycling
• Business models for the circular economy
• Battery cell production management

Homepage: https://www.uni-muenster.de/Chemie.bm/institut/vondelft.html

Selected Publications:

Core Interests:

Methodological:
• Analytical and High-Resolution Electron Microscopy
• Atomic Transport by Tracer Diffusion
• Phase Transformation Kinetics by Low- and High-temperature calorimetry

Topical:
• Structure and chemistry of electrodes and electrode/electrolyte interfaces in Lithium ion batteries
• Bulk metallic glasses: deformation, relaxation and transport kinetics
• High entropy materials: stability, microstructure evolution and functional performance

Homepage: https://www.uni-muenster.de/Physik.MP/Wilde/en/Mitarbeiter/ProfWilde.html

Selected Publications:
Core Interests:

• Solid state chemistry of ionic conductors
• Materials research for battery materials
• Interfaces in solid state batteries

Homepage: https://www.uni-muenster.de/Chemie.ac/forschung/ak_zeier/index.html

Selected Publications:


### Supervisors at MEET/HI MS

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<td>Dr. Sascha Nowak &amp; Dr. Simon Wiemers-Meyer (MEET Analytics and Environment Division)</td>
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<td>Dr. Nella Vargas-Barbosa (HI MS)</td>
<td>Ionic transport in electrolytes</td>
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All BACCARA students at MEET Battery Research Center or Helmholtz-Institute Münster will be co-advised by **Prof. Martin Winter**.
Dr. Masoud Baghernejad: Advanced Interphase Analysis

Core Interests:

Spectro-electrochemical investigation of the interphase between electrolytes and electrodes in lithium-based batteries.

- In situ/operando near-Field Raman and IR spectroscopy; technique development (core-shell nanostructures for SHINERS technique) and application for interphase investigation in lithium-based batteries,
- Interphase design and modification at electrode-electrolyte interface; synthesis of film-forming additives and electrolyte formulation (e.g. ionic liquids),
- Surface electrochemistry techniques; charge transport at the electrified interfaces.

Homepage: https://scholar.google.ch/citations?user=McAvM5EAAAAJ&hl=en

Selected Publications:

Dr. Markus Börner & Dr. Philip Niehoff (‘Cell-System’ Division)

Core Interests:

Design of Novel Batteries by Sophisticated Electrode and Cell Design, and In-Depth Understanding of Aging Effects and Safety Properties

• Development of electrode and cell designs for high power and high energy lithium ion batteries as well as lithium metal batteries and the corresponding processes
• In-depth investigation of aging effects and their remedy
• Understanding and improving safety properties of lithium ion batteries and next generation technologies

Homepage:

Cell-System Division:  https://www.uni-muenster.de/MEET/en/team/cell.html
Dr. Markus Börner:  https://www.uni-muenster.de/MEET/en/team/boerner.shtml
Dr. Philip Niehoff:  https://www.uni-muenster.de/MEET/en/team/niehoff.shtml

Selected Publications:

• Towards water based ultra-thick Li ion battery electrodes - A binder approach. *Journal of Power Sources* 2019, 423, 183–191.
• The role of the pH value in water-based pastes on the processing and performance of Ni-rich LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2 based positive electrodes. *Journal of Power Sources* 2020, 475, 228608.
• Interface investigations of a commercial lithium ion battery graphite anode material by sputter depth profile X-ray photoelectron spectroscopy. *Langmuir* 2013, 29, 5806-5816.
• Degradation effects on the surface of commercial LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2 electrodes. *Journal of Power Sources* 2016, 335, 45-55.
• Correlation of aging and thermal stability of commercial 18650-type lithium ion batteries. *Journal of Power Sources* 2017, 342, 382-392.
Dr. Peter Bieker (‘Li Metal and Beyond ‘ Group)

Core Interests:
Next Generation Batteries (NGB): Li-Metal Batteries, Magnesium, Zink and organic Batteries

• Development of stable SEI on Li metal, protection of Li by alloying, coatings, mechanical and chemical modifications
• Interphase design at electrode|electrolyte interfaces for Li II S, Li II O₂, Mg II S and Zn II Air batteries
• Designing of separator systems, membranes and hybrid electrolytes for NGB
• Design of innovative materials and cell concepts for new battery systems

Homepage:
Next Gen Group: https://www.uni-muenster.de/MEET/en/research/joint-groups/next-generation/index.html
Dr. Peter Bieker: https://www.uni-muenster.de/MEET/team/bieker.shtml

Selected Publications:
• Solid-state lithium-sulfur battery enabled by Thio-LiSICON/Ploymer composite electrolyte and sulfuized polyacrylonitrile cathode Advanced Functional Materials 2020.
Core Interests:
Design of Advanced Polymer Materials and (NMR/MRI) Methods Development

- Development of polymer materials for high capacity lithium-metal (solid-state) batteries and organic batteries (e.g., quasi-solid polymer electrolytes, multi-layered (hybrid) electrolytes, coatings of electrodes)
- Interphase design at electrode|electrolyte interfaces and understanding of charge transport phenomena (e.g., artificial SEI/CEI to prevent active lithium losses, design of cell concepts with multi-layered electrolytes)
- Design of innovative methods (NMR/MRI/EIS) and establishment of ‘descriptors’ for the analysis of batteries (e.g., NMR protocols quantification of active lithium losses, 1D MRI concentration profiling, DRT analysis)

Homepage: Helmholtz-Institute (IEK-12): https://www.fz-juelich.de/iek/iek-12/EN/AboutUs/Mitarbeiter/mitarbeiter_node.html
PD Dr. Gunther Brunklaus: https://scholar.google.de/citations?hl=en&user=-nuU_yYAAAAJ

Selected Publications:
- Quasi-solid single ion conducting polymer electrolyte membrane containing novel fluorinated poly(arylene ether sulfonimide) for lithium metal batteries J. Power Sources 2021, 484, 229267.
- Fluorinated polysulfonamide based single ion conducting room temperature applicable gel-type polymer electrolytes for lithium ion batteries. J. Mater. Chem. A 2019, 7, 188-201.
Core Interests:

- Advanced electrolyte formulations for energy storage application
- Design & synthesis of novel (multi)-functional electrolyte components
- Development of structure-property-performance relationships for understanding and elucidation of main operation and failure mechanisms
- Interface/interphase phenomena, processes and electrochemistry
- High throughput experimentation and machine learning approach for accelerated identification of affordable, electrochemically and thermally outperforming electrolytes

Homepage: https://scholar.google.com/citations?hl=en&user=5S8V2xQAAAAJ

Selected Publications:

- Fluorinated cyclic phosphorus(III)-based electrolyte additives for high voltage application in lithium-ion batteries: impact of structure–reactivity relationships on CEI formation and cell performance, ACS Applied Materials & Interfaces 2019 11 16605.
- Methyl-group functionalization of pyrazole-based additives for advanced lithium ion battery electrolytes, Journal of Power Sources 2020 461 228159.
Core Interests:

Design of Advanced Battery Materials: From Material Synthesis to Battery Cell Application

- Development of high-capacity anode and cathode materials for high energy lithium-ion batteries (e.g., Ni-rich NCM cathode materials, silicon/carbon anodes, pre-lithiation techniques)
- Interphase design at electrode|electrolyte interfaces and understanding of aging phenomena in lithium-ion cells (e.g., cross-talk phenomena, SEI degradation, active lithium loss, gassing)
- Design of innovative materials and cell concepts for inexpensive and sustainable batteries (e.g., dual-ion batteries, metal-organic frameworks, highly-concentrated electrolytes)

Homepage:  https://www.uni-muenster.de/MEET/en/research/materials/index.html
Core Interests:
Analytics and environmental aspects of lithium ion batteries and next generation materials
• Development and application of analytical method for aging investigations
• Electrolyte aging, transition metal migration, lithium loss and surface investigations
• Recycling and 2nd life of LIBs
• Potential toxicity of aging products and work safety
• Understanding and verification of the complex chemical reactions and mechanisms in a cell

Homepage: https://scholar.google.de/citations?user=gfmCsjEAAAAJ&hl=de&oi=sra
https://www.uni-muenster.de/MEET/en/team/analytics.html

Selected Publications:
• “Phytoremediation of soil contaminated with lithium ion battery active materials – A proof of concept study.” Recycling 5 (4), Special Issue: Recycling of Lithium Ion Batteries and Other Next Generation Materials: 26, 2020.
• “The role of cations on the performance of lithium ion batteries: A quantitative analytical approach.” Accounts of Chemical Research 52 (2), Special Issue: Energy Storage: Complexities Among Materials and Interfaces at Multiple Length Scales: 265-272, 2018.
Core Interests:
(Photon)electrochemistry of solid-solid and solid-liquid interfaces
• Impedance spectroscopy methods for mechanistic understanding of reactions
• Light-induced charge-transfer at electrode-electrolyte interfaces
• Hydrodynamic methods for (homogeneous/heterogeneous) electrocatalytic reactions
• Dynamics at electrode-concentrated electrolyte interfaces
• Ion transport in membranes, concentrated liquid electrolytes and solid-state electrolytes

Homepage: https://scholar.google.com/citations?user=-CxwNKsAAAAJ&hl=en

Selected Publications:
• "Understanding the Effect of Monomeric Iridium(III/IV) Aquo Complexes on the Photoelectrochemistry of IrO_x·nH_2O-Catalyzed Water-Splitting Systems” JACS, 2015, 137, 8749.