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International Graduate School BACCARA

Supervisor Guide

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BACCARA
Electrifying the Future.

Prof. Dr. Björn Braunschweig

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

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

Selected Publications:

- Kemna A, Braunschweig B, **Potential-Induced Adsorption and Structuring of Water at Pt(111) Electrode Surfaces in Contact with an Ionic Liquid .** J. Phys. Chem. Lett. 11 (2020), p. 7116-7121.
- Ratschmeier B, Kemna A, Braunschweig B, **Role of H_2O for CO_2 Reduction Reactions at Platinum/Electrolyte Interfaces in Imidazolium Room-Temperature Ionic Liquids** . ChemElectroChem 7 (2020), p. 1765-1774.
- Kemna A, García Rey N, Braunschweig B, **Mechanistic Insights on CO_2 Reduction Reactions at Platinum/[BMIM][BF_4] Interfaces from In Operando Spectroscopy** . ACS Catalysis 9 (2019), p. 6284-6292.

Prof. Dr. Nikos Doltsinis

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:

- M. Neugebauer, S. Schmitz, D. Brünink, N.L. Doltsinis, and A. Klein, **Dynamics of the efficient cyclometalation of the undercoordinated organoplatinum complex [Pt(COD)neoPh]$^+$ (neoPh=2-methyl-2-phenypropyl),** New J. Chem. 44, 19238 (2020).
- J. Bachmann, I. Schönrath, J. Müller, and N.L. Doltsinis, **Dynamic Structure and Stability of DNA Duplexes Bearing a Dinuclear Hg(II)-Mediated Base Pair,** Molecules 25, 4942 (2020).
- M. Cnudde, D. Brünink, N.L. Doltsinis, and C.A. Strassert, **Tetradentate N^N°N^N-type luminophores for Pt(II) complexes: Synthesis, photophysical and quantum-chemical investigation,** Inorganica Chimica Acta, 2020.

Prof. Dr. Melanie Esselen

Core Interests:

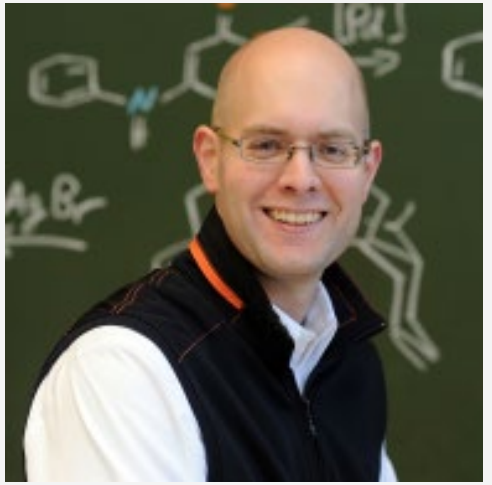
The current research of Prof. Dr. M. Esselen focuses genotoxic and mutagenic effects and combinatory toxicity of food constituents and environmental contaminants. Further, the group is interested in cell culture studies to investigate the impact of compound classes on key elements of cellular signaling 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:

- Hermes L, Römermann J, Cramer B, Esselen M. 2021. **'Quantitative Analysis of β-Asarone Derivatives in Acorus calamus and Herbal Food Products by HPLC-MS/MS.'** Journal of Agricultural and Food Chemistry 2021: Online ahead of print.
- Hermes L, Haupenthal S, Uebel T, Esselen M. 2020. '**DNA double strand break repair as cellular response to genotoxic asarone isomers considering phase I metabolism.'** Food and Chemical Toxicology 2020.
- Schultheis J, Beckmann D, Mulac D, Müller L, Esselen M, Düfer M. 2019. '**Nrf2 activation protects mouse beta cells from glucolipotoxicity by restoring mitochondrial function and physiological redox balance.'** Oxidative Medicine and Cellular Longevity 2019.

Prof. Dr. Frank Glorius



Core Interests:

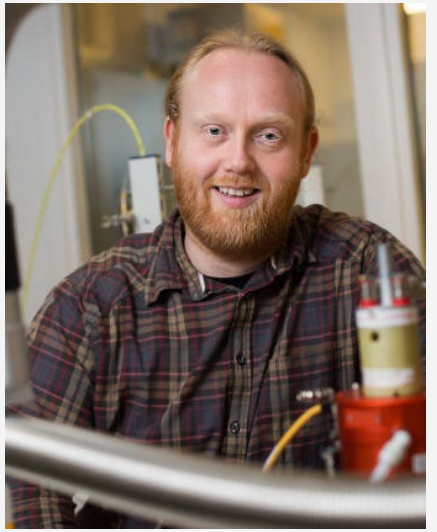
- Organic Synthesis
- N-Heterocyclic Carbenes
- Organocatalysis
- Asymmetric Catalysis
- C-H Activation
- MOFs
- Heterogeneous Catalysis
- Photoredox-Catalysis
- Smart Screening Technologies
- Electrolytes/Batteries

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

Selected Publications:

- P. Bellotti, M. Koy, C. Gutheil, S. Heuvel, F. Glorius, **Three-component three-bond forming cascade via palladium photoredox catalysis,** Chem. Sci. 2021, *12*, 1810-1817.
- T. Patra, M. Das, C. G. Daniliuc, F. Glorius, **Metal-free, photosensitized oxyimination of unactivated alkenes with bifunctional oxime carbonates,** Nature Catal. 2021, 4, 54-61.
- H.-M. Huang, P. Bellotti, C. Daniliuc, F. Glorius, **Radical Carbonyl Propargylation by Dual Catalysis**, Angew. Chem. Int. Ed. 2021, 60, 2464-2471; Angew. Chem. 2021, 133, 2494-2501.

Prof. Dr. Michael Ryan Hansen



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:

- Exner, J., Maisuls, I., Massolle, A., Klabunde, S., Hansen, M.R., Strassert, C.A., Neugebauer, J., Eckert, H., Studer, A., **Electronic effects in profluorescent benzotriazinyl radicals: a combined experimental and theoretical study** Phys, Chem. Chem. Phys. (2021).
- Radzieowski, M., Block, T., Koppe, J., Hansen, M.R., Pöttgen, R., Janka, O., **(Pseudo)binary Antimonides: Insights on Local Ordering and Effective Charge Configurations from 121Sb MAS NMR and Mössbauer Spectroscopies,** J. Phys. Chem. C 125/2, 1454–1466 (2021).
- Münster, P., Diehl, M., Frerichs, J.E., Börner, M., Hansen, M.R., Winter, M., Niehoff, P., **Effect of Li plating during formation of lithium ion batteries on their cycling performance and thermal safety,** J. Power Sources 484, 229306 (2021).

Prof. Dr. Heiko Hayen

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

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.**
- K. Scholz, A. Lipphardt, C. M Wienken, T. Tiso, H. Hayen, J. Chromatogr. A. 1631 (2020) 461584. **Hyphenation of supercritical fluid chromatography with different detection methods for identification and quantification of liamocin biosurfactants.**
- M. Baune, K. Kang, W. D. C. Schenkeveld, S. M. Kraemer, H. Hayen, G. Weber, BioMetals, 33 (2020) 305-321. **Importance of oxidation products in coumarin-mediated Fe(hydr)oxide mineral dissolution.**

Prof. Dr. Andreas Heuer

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:

- S. Tovey, A. Narayanan Krishnamoorthy, G. Sivaraman, J. Guo, C. Benmore, A. Heuer, C. Holm, **DFT Accurate Interatomic Potential for Molten NaCl from Machine Learning** J. Phys. Chem. C 124, 47, 25760–25768 (2020).
- A. Thum, A. Heuer, K. Shimizu, J.N. Canongia Lopes, **Solvate ionic liquids based on lithium bis(trifluoromethanesulfonyl)imide - glyme systemsAr: coordination in MD simulations with scales charges,** Phys. Chem. Chem. Phys. 22, 525-535 (2020).
- M. Biedermann, D. Diddens, A. Heuer, **rs@MD: Introducing Reactive Steps at the Molecular Dynamics Simulation Level,** J. Chem. Theory Comput. 17, 1074 (2021).

Prof. Dr. Hans-Ulrich Humpf

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:

- Sueck F, Specht J, Cramer B, Humpf HU. 2020. **'Identification of ochratoxin-N-acetyl-L-cysteine as a new ochratoxin A metabolite and potential biomarker in human urine.'** Mycotoxin Res. 36(1): 1-10.
- Jagels A, Stephan F, Ernst S, Lindemann V, Cramer B, Hübner F, Humpf H-U. 2020. **'Artificial vs natural Stachybotrys infestation—Comparison of mycotoxin production on various building materials.'** Indoor Air 30, No. 6: 1268-1282.
- Schulz M, Gaitanoglou V, Mantel O, Hoevelmann Y, Huebner F, Dobrindt U, Humpf HU. 2020. **'Metabolomics Study on Pathogenic and Non-pathogenic E. coli with Closely Related Genomes with a Focus on Yersiniabactin and Its Known and Novel Derivatives.'** Metabolites 10, No. 6: 221.

Prof. Dr. Joachim Jose

Core Interests:

- Autodisplay of proteins fur 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:

- Gercke, D., Furtmann, C., Tozakidis, I.E.P., Jose, J. **Highly crystalline post-consumer PET waste hydrolysis by surface displayed PETase using a bacterial whole-cell biocatalyst**, ChemCatChem 2021, 13: 1-12; doi.org/10.002/cctc.202100443
- Lenz, F., Zurek, P., Umlauf, M., Tozakidis, I.E.P., Jose, J. **Tailor-made β-glucosidase with increased activity at lower temperature without loss of stability and glucose tolerance**, Green Chemistry 2020, 22: 2234 - 2243, doi: 10.1039/c9gc04166d
- Schulte, M.F., Tozakidis, I.E.P., Jose, J., **Autotransporter-based surface display of hemicellulases on *Pseudomonas putida*: new whole-cell biocatalysts for the production of xylose from biomass**. ChemCatChem (2017), 9: 3655-3694.
- Jose, J., Meyer, T.F. **The autodisplay story – from discovery to biotechnical and biomedical applications**. Microbiol Mol Biol R (2007), 71:600-619.

Prof. Dr. Uwe Karst

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:

- Fangmeyer J, Behrens A, Gleede B, Waldvogel SR, Karst U. 2020. **'Mass-Spectrometric Imaging of Electrode Surfaces-a View on Electrochemical Side Reactions.'** Angewandte Chemie-International Edition 59, No. 46: 20428-20433.
- Scheeren SG, Fangmeyer J, Schmid R, Karst U. 2020. **'Fast Online Separation and Identification of Electrochemically Generated Isomeric Oxidation Products by Trapped Ion Mobility-Mass Spectrometry.'** Analytical Chemistry 92, No 1: 1205-1210.
- Chira R, Fangmeyer J, Zaharia V, Karst U, Bodoki E, Oprean R. 2020. **'Electrochemically Simulated Oxidative Metabolization Pattern of Neurokinin-1 Antagonist Aprepitant.'** Journal of the Electrochemical Society 167, No. 8: 085502.

Prof. Dr. Jens Leker

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:

- Duffner F, Kronemeyer N, Tübke J, Leker J, Winter M, Schmuch R. 2021. **'Post-lithium-ion battery cell production and its compatibility with lithium-ion cell production infrastructure.'** Nature Energy 2021.
- Duffner, Fabian Wentker, Marc Greenwood, Matthew Leker, Jens. 2020. **'Battery cost modeling: A review and directions for future research.'** Renewable and Sustainable Energy Reviews 127.
- Stoffels, Marius Klauck, Felix J. R. Hamadi, Thomas Glorius, Frank Leker, Jens. 2020. **'Technology Trends of Catalysts in Hydrogenation Reactions: A Patent Landscape Analysis.'** Advanced Synthesis & Catalysis 362, Nr. 6: 1258-1247.

Prof. Dr. Simon Lux

Core Interests:

- Techno-economic modelling of battery value chains incl. raw materials and sustainability
- Battery production technologies
- Materials for high temperature and high pressure applications in high voltage systems

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

Selected Publications:

- Magali Gauthier, Pinar Karayaylali, Livia Giordano, Shuting Feng, Simon F Lux, Filippo Maglia, Peter Lamp, Yang Shao-Horn. **"Probing surface chemistry changes using LiCoO2-only electrodes in Li-ion batteries."** Journal of The Electrochemical Society, 2018.
- Tianyue Zheng, Zhe Jia, Na Lin, Thorsten Langer, Simon Lux, Isaac Lund, Ann-Christin Gentschev, Juan Qiao, Gao Liu. **"Molecular spring enabled high-performance anode for lithium ion batteries."** Polymers, 2017.
- Livia Giordano, Pinar Karayaylali, Yang Yu, Yu Katayama, Filippo Maglia, Simon Lux, Yang Shao-Horn. **"Chemical reactivity descriptor for the oxide-electrolyte interface in Li-ion batteries."** The journal of physical chemistry letters, 2017.

Prof. Dr. Johannes Neugebauer

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

Selected Publications:

- J. Exner, I. Maisuls, A. Massolle, S. Klabunde, M.R. Hansen, C.A. Strassert, J. Neugebauer, H. Eckert, A. Studer, **Electronic effects in profluorescent benzotriazinyl radicals: a combined experimental and theoretical study,** Phys. Chem. Chem. Phys. 23 (2021), 2999-3007.
- X. Meng, H. Klaasen, L. Viergutz, B. Schulze Lammers, M.C. Witteler, H. Mönig, S. Amirjalayer, L. Liu, J. Neugebauer, H.-Y. Gao, A. Studer, H. Fuchs, **Azo bond formation on metal surfaces,** Angew. Chem. Int. Ed. 60 (2021), 1458-1464.
- M. Bensberg, J. Neugebauer, **Density-Functional Theory-Based Embedding Approaches for Transition-Metal Complexes,** Phys. Chem. Chem. Phys. 22 (2020), 26093-26103.

Prof. Dr. Bart Jan Ravoo

Core Interests:

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

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

Selected Publications:

- Buten C, Kortekaas L, Ravoo BJ., **Design of Active Interfaces Using Responsive Molecular Components.** Advanced Materials. 2020; 32: 1904957.
- Korshunov, A.; Gibalova, A.; Grünebaum, M.; Ravoo, B.J.*; Winter, M.*; Cekic-Laskovic, I.*, **Host-guest interactions enhance the performance of viologen electrolytes for aqueous organic redox flow batteries.** Batteries & Supercaps 2021, in press.
- Honnigfort C, Campbell RA, Droste J, Gutfreund P, Hansen MR, Ravoo BJ, Braunschweig B., **Unexpected Monolayer-to-Bilayer Transition of Arylazopyrazole Surfactants Facilitates Superior Photo-Control of Fluid Interfaces and Colloids.** Chem. Sci.. 2020; 11: 2085-2092.

Prof. Dr. -Ing. Jochen Schmid

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:

- Schilling C, Koffas M, Sieber V, Schmid J, *Novel prokaryotic CRISPR-Cas12a based tool for programmable transcriptional activation and repression*. ACS Synthetic Biology (2020), 9 (12), 3353–3363
- Schmid J, Schilling C, Badri A, Sieber V, Koffas M, Schmid J, *Metabolic engineering for production of functional polysaccharides* Current Opinion in Biotechnology (2020), 66, 44-51
- Gansbiller M, Schmid J, Sieber V, *In-depth rheological characterization of genetically modified xanthan-variants,* Carbohydrate Polymers (2019) 213, 1, 236 - 246
- 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)

Prof. Dr. Monika Schönhoff

Core Interests:

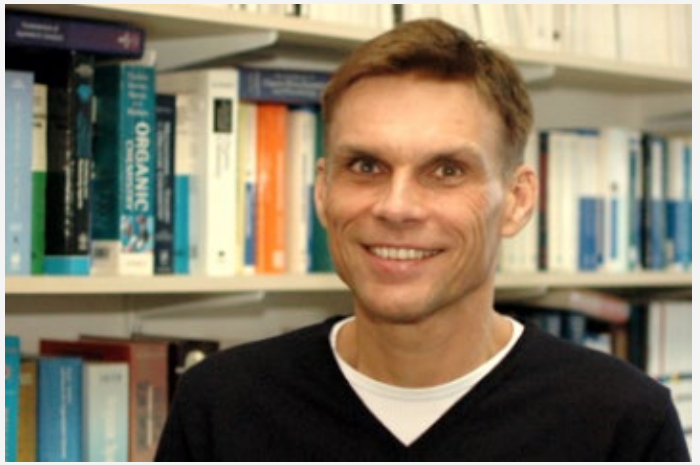
- NMR studies of molecular transport by Pulsed Field Gradient methods
- Ion transport mechanisms in battery electrolytes
- Liquid, polymeric and gel electrolytes
- Functional polymer materials from polyelectrolytes
- Porous Materials and Colloidal Carriers

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.
- Brinkkötter, M.; Mariani, A.; Jeong, S.; Passerini, S.; Schönhoff, M.; **Ionic liquid in Li Salt Electrolyte: Modifying the Li+ Transport Mechanism by Coordination to an Asymmetric Anion,** Adv. Energy Sustainability. Res. 2021, 2, 2000078.
- Pfeifer, S.; Ackermann, F.; Sälzer, F.; Schönhoff, M.; Roling, B.; **Quantification of Cation-Cation, Anion-Anion and Cation-Anion Correlations in Li Salt/Glyme Mixtures by combining Very-low-frequency Impedance Spectroscopy and Diffusion and Electrophoretic NMR,** Phys. Chem. Chem. Phys. 2021, 23, 628-640.

Prof. Dr. Armido Studer



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:

- **Electronic effects in profluorescent benzotriazinyl radicals: A combined experimental and theoretical study,** J. Exner, I. Maisuls, A. Massolle, S. Klabunde, M. R. Hansen, C. A. Strassert, J. Neugebauer, H. Eckert, A. Studer, Phys. Chem. Chem. Phys. 2021, 23, 2999-3007.
- **Functionalization of α-C(sp3)–H Bonds in Amides Using Radical Translocating Arylating Groups,** N. Radhoff, A. Studer, Angew. Chem. Int Ed. 2021, 60, 3561-3565.
- **Azo bond formation on metal surfaces**, X. Meng, H. Klaasen, L. Viergutz, B. Schulze Lammers, M. C. Witteler, H. Mönig, S. Amirjalayer, L. Liu, J. Neugebauer, H.-Y. Gao, A. Studer, H. Fuchs, *Angew. Chem. Int. Ed.* 2021, *60*, 1458-1464.

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:

- von Delft Stephan, Zhao Yang. 2021. **'Business models in process industries: Emerging trends and future research.'** Technovation, 102195.
- Zhao Yang, von Delft Stephan, Morgan-Thomas Anna, Buck Trevor. 2020. **'The evolution of platform business models: Exploring competitive battles in the world of platforms.'** Long Range Planning 53, Nr. 4.
- von Delft Stephan, Gelhard Carsten, Kortmann Sebastian, Pisani Niccolò. 2019. '**Leveraging global sources of knowledge for business model innovation.'** Long Range Planning 52, Nr. 5.

Prof. Dr. Gerhard Wilde

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:

- Jingfeng Zhang, G Mohan Muralikrishna, Alex Asabre, Yordan Kalchev, Julian Müller et al. 2021. **'Tracer diffusion in the σ phase of the CoCrFeMnNi system.'** Acta Materialia 203.
- A. Davani F, Hilke S, Rösner H , Geissler D, Gebert A, Wilde G. 2020. **'Correlations between the ductility and medium-range order of bulk metallic glasses.'** Journal of Applied Physics 2020, No. 128.
- A. Davani Farnaz, Hilke Sven, Rösner Harald, Geissler David, Gebert Annett, Wilde Gerhard. 2020. **'On the shear-affected zone of shear bands in bulk metallic glasses.'** Journal of Alloys and Compounds 837.

Prof. Dr. Wolfgang Zeier

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:

- Ohno S., Rosenbach C., Dewald G.F., Janek J., Zeier W.G., "**Linking Solid Electrolyte Degradation to Charge Carrier Transport in the Thiophosphate-Based Composite Cathode toward Solid-State Lithium-Sulfur Batteries**" Adv. Funct. Mater. 2021.
- Culver S.P., Squires A.G., Minafra N., Armstrong C.W.F., Krauskopf T., Böcher F., Li C., Morgan B.J., Zeier W.G., **"Evidence for a Solid-Electrolyte Inductive Effect in the Superionic Conductor Li10Ge1-xSnxP2S12"** J. Am. Chem. Soc. 2020, 142, 21210-21219.
- Schlem R., Banik A., Ohno S., Suard E., Zeier W.G., "**Insights into the Lithium Sub-structure of Superionic Conductors Li3YCl6 and Li3YBr6"** Chem. Mater 2021.

Overview of possible BACCARA supervisors at MEET and HI MS

Supervisors at MEET/HI MS	Area of Research
Dr. Masoud Baghernejad (HI MS)	Spectro-electrochemical investigation of the interphase between electrolytes and electrodes
Dr. Markus Börner & Dr. Philip Niehoff (MEET Cell System Division)	Sophisticated Electrode and Cell Design, understanding of Aging Effects and Safety Properties
Dr. Peter Bieker (MEET Focus Group Next Generation)	Next generation Batteries
PD Dr. Gunther Brunklaus (HI MS)	Advanced Polymer Materials, NMR/MRI Methods Development
Isidora Cekic-Laskovic (HI MS)	
Dr. Johannes Kasnatscheew (MEET Materials Division)	Materials Synthesis, Interphase Design, Electrochemistry
Dr. Kerstin Neuhaus	Solid state ionics and AFM-based electrochemical methods
Dr. Sascha Nowak & Dr. Simon Wiemers-Meyer (MEET Analytics and Environment Division)	Analytics, Recycling, 2nd Life, Aging

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:

- Jonas H.K. Pfisterer, Masoud Baghernejad, Giovanni Giuzio, Katrin F Domke (2019): *'Reactivity mapping of nanoscale defect chemistry under electrochemical reaction conditions.' Nature Communication*, 10, 5702.
- Masoud Baghernejad, Wenjing Hong*, Peter Broekmann, Thomas Wandlowski, Kristian S. Thygesen*, Martin R. Bryce* (2014): 'Electrochemical control of single-molecule conductance by Fermi-level tuning and conjugation switching.' *Journal of the American Chemical Society*, 136, 17922.
- Hao Yin, Li-Qing Zheng*, Wei Fang, Guillaume Goubert, Hua Zhang, Hai-Sheng Su, Bin Ren, Jeremy O. Richardson*, Jian-Feng Li*, Renato Zenobi*. Nanometre-scale spectroscopic visualization of catalytic sites during a hydrogenation reaction on a Pd/Au bimetallic catalyst. Nat. Catal., 2020, 3, 834.

Dr. Markus Börner & Dr. Philip Niehoff (‚Cell-System' Division)

Markus Börner

Philip Niehoff

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

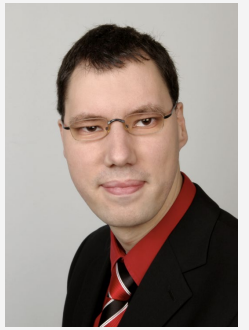
Homepage:

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)



Peter Bieker

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 O_2, Mg II S and Zn II Air batteries
- Designing of separtor systems, membrans 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:

- Galvanic Corrosion of Lithium-Powder-Based Electrodes.' *Advanced Energy Materials* 2020.
- Solid-state lithium-sulfur battery enabled by Thio-LiSICON/Ploymer composite electrlyte and sulfuized polyacrylonitrile cathode *Advanced Functional Materials 2020.*
- High Capacity Utilization of Li Metal Anodes by Application of Celgard® Separator-Reinforced Ternary Polymer Electrolyte.' *Journal of The Electrochemical Society* 2019 166, Nr. 10: A2142-A2150.

PD Dr. Gunther Brunklaus (‚Electrolytes', ‚Methods'))

Gunther Brunklaus

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:

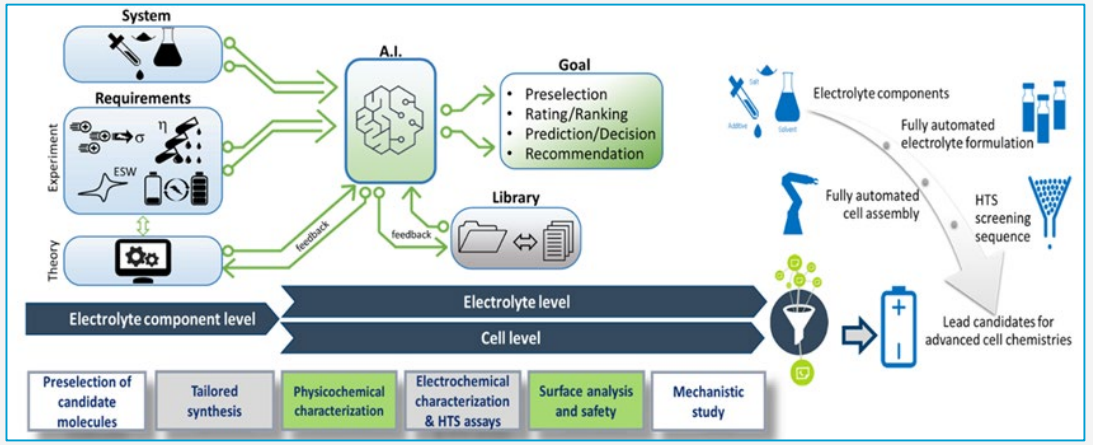
- Lithium metal polymer electrolyte batteries: opportunities and challenges. *Electrochemical Society Interface* **2019**, 28, 55-61.
- Quasi-solid single ion conducting polymer electrolyte membrane containing novel fluorinated poly(arylene ether sulfonimide) for lithium metal batteries *J. Power Sources* **2021**, 484, 229267.
- Quantification of Dead Lithium via In Situ Nuclear Magnetic Resonance Spectroscopy. *Cell Reports Physical Science* **2020,** 1, 100139.
- 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.
- Small Groups, Big Impact: Eliminating Li+ Traps in Single-Ion Conducting Polymer Electrolytes. *iScience* **2020**, 23, 101417.
- Revealing the Impact of Film-Forming Electrolyte Additives on Lithium Metal Batteries via Solid-State NMR/MRI Analysis. *J. Phys. Chem.* **2021**, 125, 252-265.

Dr. Isidora Cekic-Laskovic

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:

- Fluorine and lithium: ideal partners for high-performance rechargeable battery electrolytes, Angewandte Chemie Int. Ed. **2019** *58* 2.
- 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.
- An oxo-verdazyl radical for a symmetrical non-aqueous redox flow battery, Journal of Materials Chemistry A, **2020** *8* 22280.

Dr. Johannes Kasnatscheew (‚Materials' Division)

Core Interests:

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

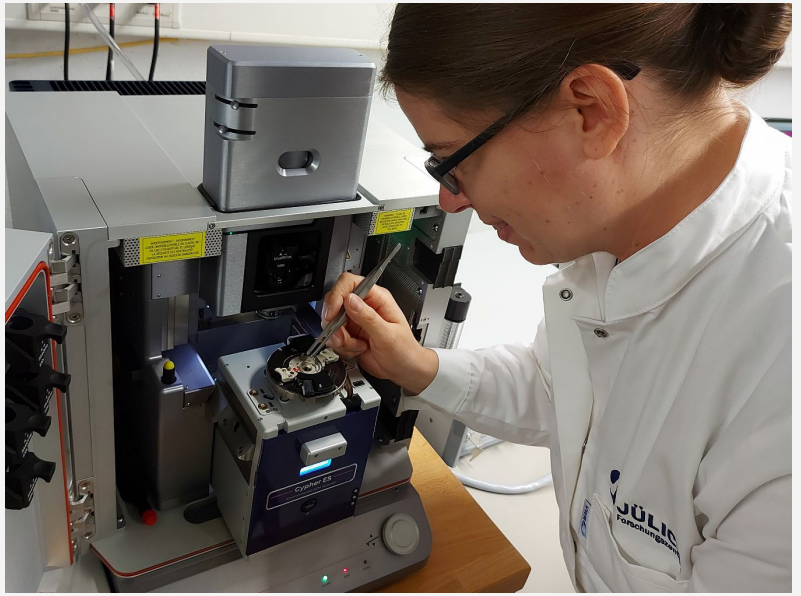
- Development of high-capacity anode and cathode materials for high energy lithium-ion batteries (e.g., Ni-rich NCM cathode materials, silicon/carbon anodes, pre-lithiation techniques)
- Interphase design at electrode|electrolyte interfaces and understanding of aging phenomena in lithium-ion cells (e.g., 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/team/materials.shtml

Selected Publications:

- "Understanding the Outstanding High-Voltage Performance of NCM523||Graphite Lithium Ion Cells after Elimination of Ethylene Carbonate Solvent from Conventional Electrolyte." Advanced Energy Materials 11, 2003738, 2021.
- "Single-Ion versus Dual-Ion Conducting Electrolytes: The Relevance of Concentration Polarization in Solid-State Batteries." ACS applied materials & interfaces 14, Nr. 9: 11559–11566, 2022.
- "Prospects and Limitations of Single-Crystal Cathode Materials to Overcome Cross-Talk Phenomena in High-Voltage Lithium Ion Cells." Journal of Material Chemistry A, Nr. 9, 7546-7555 2021.

Dr. Kerstin Neuhaus



Core Interests:

- Electrochemical measurements of ion conductive ceramic materials
- Optimization and application of AFM-based electrochemical techniques to characterize interfaces
- Development of oxide-based ceramic materials for energy storage applications

Homepage: https://www.fz-juelich.de/profile/neuhaus_k

Selected Publications:

- K. Neuhaus, C. Schmidt, L. Fischer, W.A. Meulenberg, K. Ran, J. Mayer, S. Baumann: *Measurement of polarization effects in dual-phase ceria-based oxygen permeation membranes using Kelvin Probe Force Microscopy*, Beilstein J. Nano 12 (2021) 1380-1391

- A. Buchheit, M. Hoffmeyer, B. Teßmer, K. Neuhaus: *Characterization of the Particle-Polymer Interface in Dual-Phase Electrolytes by Kelvin Probe Force Microscopy*, J. Electrochem. Soc. 168 (2021) 010531

Dr. Simon Wiemers-Meyer & Dr. Sascha Nowak (‚Analytics & Environment' Division)

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 prodcuts 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:

- "Clarification of decomposition pathways in a state-of-the-art lithium ion battery electrolyte through 13C-labeling of electrolyte components." Angewandte Chemie International Edition 59, Nr. 15: 6128-6137, 2020.
- "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.