Factbook Chemistry Graz

Basic Information about Chemistry Research Groups
at TU Graz and Uni Graz at a Glance

As of September 2024

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Preface

It is with great pleasure that we present the **Factbook Chemistry Graz**, a product of the collaborative efforts initiated during the joint external evaluation of the chemistry departments at the University of Graz and Graz University of Technology in November 2023. The primary objective of this evaluation was to explore new opportunities for collaboration and to enhance synergies within the field of chemistry research.

The **Factbook** provides a comprehensive collection of fact sheets, each highlighting a chemistry research group from one of our institutions. These sheets offer valuable insights, including an overview of the group's research focus, a summary of available instrumentation, and essential contact information. We envision this resource as a tool to foster the identification of overlapping expertise, facilitate access to specialized equipment, and, ultimately, inspire new collaborative ventures within the chemistry community.

For the most neutral representation possible, all contributions have been randomly sorted.

We want to express our sincere gratitude to everyone who contributed to the creation of this **Factbook**. We hope it will serve as a valuable resource for nurturing partnerships and driving forward the boundaries of chemistry research of the chemistry groups at our two Universities in Graz.

Profs. Jörg Feldmann and Martin Wilkening
On behalf of NAWI Graz

Gescheidt Group

Univ.-Prof. Georg Gescheidt-Demner

http://www.ptc.TUGraz.at/gescheidt/

Research abstract

We investigate chemical reactivity involving paramagnetic species (radicals and transition-metal ions) and photo induced reactions. Beside basic research on structures of intermediates products and, in particular, transient species and kinetics we address projects connected to (industrial) photopolymerization (3D printing) and catalysis.

The focus is on improving experimental conditions and making chemical reactions more efficient. Moreover, we develop photo-based NMR spectroscopy.

We use optical spectroscopy (time resolution down to the ns range), (photo) NMR (photo) CIDNP, EPR, voltammetry.

Relevant scientific infrastructure

- EPR benchtop
- EPR X-band with temperature control and irradiation
- X-Band ENDOR
- NMR/CIDNP 200 MHz (2x)
- NMR (photo) 400 MHz
- Laser-flash photolysis
- Cyclovoltammetry

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Materials for Renewable Energy

Univ.-Prof. Gregor Trimmel

https://www.tugraz.at/institute/ictm/research/trimmel-group

Research abstract

1. Synthesis and characterisation of new materials – functional polymers, organic dyes, non-fullerene acceptors, metal sulfides, tin perovskites and inorganic-organic hybrid materials
2. Organic solar cells and perovskite solar cells - materials, devices and stability of devices
3. Metal sulfide thin layers as photocatalysts for hydrogen production – synthesis of nanoparticles, porous thin films and development of new precursors for metal sulfides
4. Shape memory materials and elastomer technology

References

- Elena Zuccalà, Suman Malllick, Lea-Marie Habich, Heinz Amenitsch, Thomas Rath, Gregor Trimmel, New J. Chem., 2024, 48, 3974-3983. https://doi.org/10.1039/D3NJ05560D
- Reinhold Pommer, Robert Saf, Ralf Supplit, Armin Holzner, Harald Plank, Gregor Trimmel, Polymer, 2023, 284, 126302; https://doi.org/10.1016/j.polymer.2023.126302
- Peter Fürk, Suman Mallick, Thomas Rath, Matiss Reinfelds, Mingjian Wu, Erdmann Spiecker, Nikola Simic, Georg Haberfehlner, Gerald Kothleitner, Barbara Ressel, Sarah Holler, Jana B. Schaubeder, Philipp Materna, Heinz Amenitsch and Gregor Trimmel; J. Mater. Chem. C, 2023, 11, 8393-8404; https://doi.org/10.1039/D3TC01112G
- Eftyhmia Vakalopoulou, Daniel Knez, Marco Sigl, Gerald Kothleitner, Gregor Trimmel, Thomas Rath ChemNanoMat 2023, 9, e202200414; https://doi.org/10.1002/cnma.202200414

Relevant scientific infrastructure

- Perkin Elmer DSC 8500 – Differential Scanning Calorimeter (temperature range -50 °C to 450 °C)
- JMS-T2000GC AccuTOF™ GC-Alpha High Performance Gas Chromatograph- Time-of-Flight Mass Spectrometer (JEOL) (Kontakt: Robert Saf)
- Perkin Elmer Thermogravimetric Analyzer TGA 8000 – GC (Shimadzu GC-2010 Plus) – MS (Shimadzu GCMS-QP2010 SE)
- Gel permeation chromatography systems (various, THF and chloroform as solvent)
- Surface Profiler (Bruker Dektak XT, NAWI Graz infrastructure)
- Digital Optical Microscope (Olympus DSX1000)
- Benchtop Powder X-ray Diffractometer (Rigaku MiniFlex)

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Hanzu Group

Assoc.Prof. Ilie Hanzu

https://www.tugraz.at/institute/ictm/research/hanzu-group

Research abstract

Advanced battery materials. Hanzu group focusses on battery materials for advanced electrochemical energy storage systems. While Li-ion technology is in the main focus, materials for alternative systems, such as sodium-ion batteries are also actively developed and investigated. Understanding structure-property relations is one key goal of our work. The expertise in the group ranges from materials synthesis to the fundamental processes related to ion storage and transport in active materials, as well as in liquid and hybrid (solid) electrolytes, *e.g.* based on MOF-ionic liquids composites. The stability of electrochemical interfaces in battery materials and battery ageing phenomena are within the competences of the group. On request, we offer scientific consulting on battery technology and we conduct complex and accurate active materials testing on samples supplied by our industrial partners. Nanomaterials synthesis by anodization (electrochemical oxidation), as well as electrodeposition of porous materials, such as MOFs (Metal Organic Frameworks), are two secondary topics of the group.
Methods: a broad range of advanced electrochemical techniques, battery cycling techniques, cyclic voltammetry, GITT (Galvanostatic Intermittent Titration Technique), PITT (Potentiostatic Intermittent Titration Technique), EIS (Electrochemical Impedance Spectroscopy) in the liquid state, X-ray diffraction, entropymetry.

Keywords: battery materials, electrochemistry, non-aqueous electrolytes, hybrid electrolytes, battery electrode preparation, test cell assembly, electrochemical interfaces in batteries, battery ageing, *in operando* spectroscopy, layered cathodes, lithium iron phosphate, hard carbons, titania nanotubes, nano-materials, anodization, electrodeposition.

Recent examples:

N. Šimić, A. Jodlbauer, M. Oberaigner, M. Nachtnebel, S. Mitsche, H.M.R. Wilkening, G. Kothleitner, W. Grogger, D. Knez, I. Hanzu, Phase Transitions and Ion Transport in Lithium Iron Phosphate by Atomic-Scale Analysis to Elucidate Insertion and Extraction Processes in Li-Ion Batteries, *Advanced Energy Materials*, 14 (2024) 2304381. Link

A. Ferbezar, R. Zettl, K. Hogrefe, H. Fitzek, B. Gadermaier, H.M.R. Wilkening, I. Hanzu, Tuning the ion conductivity of Zr-based metal–organic framework ionogels by linker functionalization, *Journal of Materials Chemistry A*, 12 (2024) 12552-12563. Link

Relevant scientific infrastructure

- ECC-Opto-10 electrochemical cells for *in operando* Raman spectroscopy (sapphire window) and X-ray diffraction experiments (beryllium window).
- Battery cyclers: VMP3 (12 channels), MPG2 (16 channels), MACCOR 4000 (40 channels).
- High voltage (100 V) potentiostat/ galvanostat and anodization cells for titania nanotubes synthesis.
- Portable potentiostat/ galvanostat (SP 50, BioLogic).
- Ar filled gloveboxes.
- Test cells (Swagelok, coin cells, pouch cells) and cell assembly equipment.
- Temperature controlled baths and ovens for ageing studies.
- Custom designed electrochemical cells for MOF electrodeposition.

Equipment shared with Prof. Wilkening Group

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TESLA – Trace Element Speciation Laboratory for Environmental Chemistry

Univ.-Prof. Jörg Feldmann

https://analytische-chemie.uni-graz.at/en/research/tesla/

Research abstract

The TESLA group is interested in trace and **ultra-traces** of elements (mainly **arsenic, mercury, selenium** and **fluorine**) and their molecular transformation in biological, environmental and technical processes. We are interested in describing **environmental processes** by developing **novel analytical approaches** for the elements in question. Here we focus on their molecular diversity of **natural compounds and emerging contaminants** including nano and microparticles in bulk samples as well as with spatial resolution at the micrometre level.

Main topics:

- Mercury contamination in the **off-shore oil and gas infrastructures** such as pipelines and its impact on the biomagnification in the marine food chain
- Mercury detoxification process in stranded whales by forming **mercury/selenium nanoclusters** and their distribution and translocation in their tissues
- Characterisation of multi-element fingerprint of **natural nanoparticles** in whale livers using ICP-TOFMS (collaboration with David Clases)
- Effects of **engineered NPs** on the uptake of mercury, arsenic and PFAS by plants
- Identification of **fluorinated microparticles** from bulk polymers (collaboration with David Clases)
- Mercury contamination in historic lighthouses in Britain and Ireland before and after restauration
- Multiplatform analytical approaches to determine **PFAS in ski wax** and their distribution in Alpine soil and groundwater
- **Fluorinated pesticides and pharmaceuticals** in sewage water and its destruction by UV and ozone.
- PFAS and a **fluorine mass balance** in tissues from non-contaminated wildlife at different trophic level (wild boars (CZ), deer (D), chamois (A), bees (A), whales (Brazil & UK))
- Target and non-target **PFAS in atmospheric depositions** (PM10 and water/snow) at remote stations in Germany (from the North Sea to the Alps) over 2 years
- **Ozone treatment on PFAS** in sewage water and its destruction to ultra-short chain PFAS (TFA etc.)
- Development of **novel ionisation sources** for non-polar PFAS in liquid samples with elemental and molecular mass spectrometric detection (CAM, ICPMS, ...)
- Measurements of non-polar and polar PFAS using NMR and MS methods (collaboration with K. Zangger)
- Development of field kits for **inorganic arsenic in rice** and survey of arsenic loaded rice in Europe

Relevant scientific infrastructure

- Separation of Nano and microparticles with general and element-specific detection with asymmetric flow field flow fractionation: **AF4-MALS-ICPMS**
- PFAS non-targeted analysis with high resolution molecular mass spectrometry with liquid chromatography: **HPLC-ESI-qTOF-MS**
- Total Fluorine analysis in solid and liquid samples with combustion ion chromatography: **CIC**
- Element-specific detection with coupled liquid chromatography especially for fluorine: **HPLC-ICPMS**
- Imaging at the micrometre scale of trace elements in biological, geological and technical material using laser ablation: **LA-ICPMS**
- Determination of non-polar and volatile PFAS using gas chromatography coupled to atomic emission spectrometry: **GC-AED**
- Ultra-trace mercury detection in biological and technical samples using atomic fluorescence: **CV-AFS**

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Element Analysis and Applied Atomic Spectrometry

Dr. Helmar Wiltsche

https://www.tugraz.at/institute/acfc/research/elementanalysis

Research abstract

- New instrumentation for high-pressure (40 bar) microwave-heated flow digestion
- Radio-frequency (RF) heated sample digestion
  In literature volumetric heating of mineral acids in the microwave field is postulated. Recent work of the element analysis and applied atomic spectrometry group proved this hypothesis wrong. Much to the contrary the penetration depth of microwave radiation in highly conductive liquids such as mineral acids used for sample digestion is below 1 mm. Based on these results, the aim of the RF-heated sample digestion project is to attain volumetric heating by drastically reducing the frequency of the electromagnetic radiation used to heat the sample/acid mixture.
- Application of microwave induced plasma (MIP) sources to atomic spectrometry
  - MIP-OES: For about 5 years, emission spectrometry employing MIPs received great attention in the literature. Contrary to most reports, we employ a simultaneous spectrometer for this purpose, allowing us to study matrix effects of easily ionisable elements in detail and on a large number of emission lines.
  - MIP-MS: Work on interfacing an MIP to a mass spectrometer is currently been performed. Contrary to the available literature, a collision/reaction cell is intended to be used to control interferences in the low mass region. It is interesting to note, that although nitrogen plasmas such as the MICAP (microwave-sustained, inductively coupled plasma) has an inherently lower ionization efficiency, the much lower mass of nitrogen compared to argon can be expected to result in a drastic reduction of polyatomic interferences in the analytically important mass range between 35 - 80 amu. In this respect it is also envisioned to optimize the MICAP - mass spectrometer interface geometry, as it is evident from the large difference in sonic speed of argon and nitrogen, that at least the distance between sample- and skimmer cone needs to be optimized for maximal ion throughput.
  - Tandem-MIP: Research on a novel tandem-MIP is currently underway. Tandem plasmas are plasma sources having two spatially separated plasma toroids. Though these toroids are separated, they are in comparatively close proximity. The aerosol containing the analyte is introduced into the first plasma toroid. There mostly drying of the aerosol droplets and matrix decomposition takes place. The analyte then passes to the second plasma toroid, where dominantly the excitation and ionization occurs. At least in theory, by having two distinct plasma sources coupled together, the drying / matrix decomposition and analyte excitation / ionization can be optimized independently and without the compromises typical for the ICP: in ICP-OES it is well known, that low plasma power results in reduced plasma continuum and thereby in improved LODs. However, under these conditions the plasma robustness is decreased making the ICP more susceptible to matrix effects. Having two spatially separated plasmas, allows for high RF power in the first discharge, whereby effects of the sample matrix can be reduced, while the second discharge could be driven at lower power for reduced plasma continuum. While in principle tandem plasmas have been recognized as promising alternative to classical analytically used plasma discharges, the actual construction is very difficult, indeed.

Relevant scientific infrastructure

- ICP-OES: Arcos II (Spectro, Germany), Ciros (Spectro, Germany)
- ICP-MS: NexION2000 (PerkinElmer, USA), ElanDRC+ (PerkinElmer, USA)
- HR-ICP-MS: Element2 (Thermo Fisher Scientific, USA)

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Computational Chemistry

Ao. Univ.-Prof. Anne-Marie Kelterer

http://www.ptc.tugraz.at/kelterer/

Research abstract
Computational Chemistry in the FoE Advanced Materials Science: • Material characterization and material design applying model chemistry and quantum chemistry; • Photophysical properties of organic dyes, drugs and photoinitiators; computational spectroscopy; • Structure and thermodynamic properties of solvents, and solvent effects for materials modeling. • Density functional theory and post - Hartree Fock methods.

Relevant scientific infrastructure
Software Licenses for Computational Chemistry: AMBER (MD code; group license) Gaussian16 (quantum chemistry suite; TU Campus License)

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NanoMicroLab

Ass.-Prof. David Clases

https://analytische-chemie.uni-graz.at/en/research/nulab/

Research abstract
We focus on the development of methods to characterise structures with dimensions at the nano- and microscale. Our main tool is inductively coupled plasma – mass spectrometry, which we employ in "single particle" and "imaging" mode. The former allows us to count individual particles and determine number concentrations, sizes and compositions. The latter uses a hyphenated laser ablation system, which allows the resolution of the two-dimensional element distribution. Using in-house manufactured standards, we also calibrate the concentration of elements in the resulting maps. Overall, we aim to gain a detailed look at small structures in biological and environmental systems. This includes for example anatomical microstructures in biological tissues, small features in geological samples but also individual nano- und microparticles in complex environments including micro/nanoplastics, natural mineral particles as well as anthropogenic nanocontaminants.

Relevant scientific infrastructure

- ICP-TOFMS (Nu Vitesse)
- Laser ablation (193 nm Excimer laser)
- Optical trap with Raman module (OF2i-Raman)

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Chemical Sensors and Biosensors

Assoc. Prof. Sergey Borisov & Assoc. Prof. Torsten Mayr

https://www.tugraz.at/institute/acfc/research/chemical-sensor-and-biosensors

Research abstract

Our research is dedicated to all aspects of sensors based on optical transduction including dyes, sensing materials, read-out systems and applications. Optical sensors (optodes) are characterized by absence of electromagnetic interferences, comparably low cost, variety of formats (planar sensors, fiber-optic (micro)sensors, nanoparticles etc.), minimally invasive character, suitability for miniaturization, which makes them a promising alternative to more conventional analytical techniques. However, reliable quantification of vital parameters such as oxygen, pH, acidic and basic gases, ions, glucose etc. is only possible with help of advanced materials which combine high selectivity, good brightness, excellent chemical and photochemical stability and therefore, the main research topics, on one hand, include synthesis and characterization of novel luminescent indicators, fabrication of high performance sensing materials and optical sensors but also design of dedicated read-out devices and optical components. On the other hand, numerous applications of these sensors in biotechnology, medicine, biology, environmental monitoring and other fields are realized together with collaboration partners from academia and industry.

Relevant scientific infrastructure

- Synthetic and purification equipment: Advion Benchtop Massspec, Biotage Select Flash Chromatography, Anton Paar Monowave 50 synthesis reactor, planet ball mill
- Spectroscopic equipment: Horiba Fluorolog 3 Fluorescence spectrometer with TCSPC, 2 Hitachi 7000 Fluorescence Spectrometers, Agilent Spectrophotometers, Stanford Research Lock-in Amplifier, BMG Labtech Microplate reader
- Luminescence Imaging equipment: PCO FLIM Camera, PCO SensiCam, Omicron LED-HUB
- Particle Size Analyzer: Malvern

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The Falcaro Group

Univ.-Prof. Paolo Falcaro

https://www.tugraz.at/institute/ptc/research/the-falcaro-group

Research abstract

The Falcaro group specializes in the development and application of porous materials, particularly metal-organic frameworks (MOFs) intersecting nanotechnology, crystal engineering, and materials science and biotechnology. The group explores various advanced material synthesis techniques, including self-assembly, sol-gel processes, film deposition, and patterning.

A significant portion of the Falcaro group work aims at the use of MOFs for biomedical applications and biocatalysis, including the encapsulation of enzymes, proteins, and DNA to protect their activity from environmental fluctuations, such as temperature changes. This encapsulation technology has promising applications in drug delivery, biocatalysis, and other biotechnological processes.

Additionally, the group is developing protocols to control the crystal engineering of MOFs where controlled crystal growth and orientation are crucial for achieving directionally dependent properties.

MOF engineering is applied to biotechnology, sensing, environmental remediation, and device fabrication.

Relevant scientific infrastructure

- Asylum Research Cypher VRS Atomic Force Microscope (AFM)
- Micromeritics 3flex (BET)
- Thermo Scientific™ DXR™ 2 Raman Microscope
- Rigaku SmartLab high-resolution X-ray diffractometer (XRD)
- Bruker Alpha FTIR
- Thermo Scientific NanoDrop One UV-Vis
- Zeiss Axio Scope A1 optical microscope
- Biolin Scientific KSV Nima Multi Vessel Dip-Coater
- Laurell WS-650-23B Spin Coater
- Biolin Scientific KSV Nima Langmuir-Blodgett

The complete list with descriptions and specifications is available here:
https://www.tugraz.at/institute/ptc/research/the-falcaro-group/equipment

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Sustainable Bioorganic Synthetic Chemistry

Assoz. Prof. Mélanie Hall

http://biocatalysis.uni-graz.at/

Research abstract
We are dedicated to advancing environmentally friendly, bio-based synthetic processes that prioritize sustainability and safety in organic chemistry. By leveraging the catalytic power of enzymes, we develop innovative solutions that significantly reduce energy consumption, minimize the reliance on harmful chemicals, and decrease waste. Our research is focused on pioneering non-natural reactions through the use of natural biocatalysts and on generating optically active molecules with exceptional selectivity. We are increasingly interested in integrating modern computational methods to enhance our expertise in molecular biology, organic synthesis, and the characterization of organic molecules. We actively seek collaborations, particularly in the areas of molecular docking simulations, genomics, and transcriptomics, to broaden the impact of our work and explore new frontiers in sustainable chemistry.

Relevant scientific infrastructure
• Cf Infrastructure of **Biocatalytic Synthesis**

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Spectroscopy and Electrochemistry

Ao. Univ.-Prof. Stephan Landgraf

http://www.cecp.at/index.php/about/member-pages/landgraf

Research abstract

Weak effects on electron transfer reactions
  Magnetic field effects, Solvent properties and mixtures

Photochemical Methods
  Application of semiconductor light sources, fluorescence standards (IUPAC), electron transfer theory

Pure and applied electrochemistry
  Electrochemical methods, Kinetics and Ionic liquids

Relevant scientific infrastructure

- MARY apparatus, measurement of the fluorescence signal (I) or of dI/dB as a function of the magnetic field B, TCSPC (excitation 267nm to VIS) in the normal mode/inverted mode/MSA in the magnetic field (-200 to 6000 G), cooled PMTs (down to -30 °C), temperature-controlled sample holder (5 to 70 °C)
- Solvent Lab, measurement of the solvent dielectric constant, real part, oscillator circuit, or direct capacitance method, molecular dipole moment (via temperature dependent dielectric constant), solvent density, viscosity, and refractive index, 589 nm or others (all 5 to 70 °C), using automated methods
- Modulation fluorometry (LD/LED, excitation 310 nm to NIR), <100 ps resolution
- TCSPC, inverted mode (LD/LED, excitation 267 to 635 nm) and MSA, digital delay, <50 ps resolution
- Fluorimeter Horiba FluoroMax (Calibrated I/λ), with cooled detector, all methods with temperature-controlled sample holders (5 to 70 °C), external fluorescence measurements via light guides (-30 to +300 °C)
- UV/VIS spectrophotometer Hach Lange DR5000, 190-1100 nm
- Physical light intensity measurements with calibrated detectors, Newport
- Detector system intensity calibration with calibrated lamp (W, 250 to 2000 nm)
- Detector system wavelength calibration with calibrated lamp (Hg-Ar, 185 nm to NIR)
- Diode array spectrometer (180 to 880 nm, Ocean Optics Flame)
- Absolute fluorescence quantum yield measurement of solid and liquid samples, integrating sphere
- (Mini-)cyclic voltammetry, rotating disc electrodes and impedance measurements (0.5 to 50 ml, 5 to 70 °C)
- VersaStat 3 and µAutoLab III/FRA2 potentiostat
- Oxygen sensor for high-purity gases (Lambda) and high concentrations (Clark)
- pH, redox, and conductivity measurements (5 to 70 °C), spectroelectrochemistry
- Hoffmann voltammeter and electrochemical water splitter

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Chemistry and Technology of Biobased Systems (IBioSys)

Univ.-Prof. Tanja Wrodnigg, Univ.-Prof. Karin Stana Kleinschek TU Graz

https://www.tugraz.at/en/institutes/ibiosys/home

Research abstract

The research activities of the Institute of Chemistry and Technology of Biobased Systems, IBioSys, amalgamate two main research fields with a common interest "Biobased Systems" – bioactive glycoconjugates.

Chemistry of Biobased Systems | Design and development of efficient and economic synthetic methods for bioactive glycoconjugates and analogues as well as glycomimetics based on renewable resources and their application as potential tools for the profiling as well as structure-activity-studies of glycoprocessing enzymes and as therapeutics for the management of diseases related to carbohydrate metabolism. Design, synthesis, modification and characterisation of biobased systems such as oligo- and polysaccharides for medicinal applications as well as application in material technologies such as 3D printing technologies, tissue engineering, coating technologies, fabrication of surface-active materials, applications or auxiliary materials for paper- and pulp industry.

Technology of Biobased Systems | Development of complex materials, conjugates based on biomolecules of living organism origin and analogues. This implements the manufacturing, analysis and application of organic structures and inorganic/organic hybrid-systems. The focus is set on the development of biomaterials with emphasis on surface specific processes (surface functionalisation) and manufacturing of 3D structured materials and using modern technology as 3D printing or laser lithography, development of bio-inks formulations, cross linking - and self-assembly structures, for as example tissue engineering. Another research topic is the use of mono-, oligo- and polymers and derivatives for different technical applications such as packaging, paper conservation, paper process technology, textile industry, coating or cosmetics.

Relevant scientific infrastructure

- Homogenizer (GEA: Panther)
- 3D Bioprinter GeSiM: BioScaffolder BS 3.2
- GC-MS (PerkinElmer: CLARUS 580 and SQ 8)
- FDM 3D Printer (Creality: Ender 3 V2)
- Resin 3D Printer (ANYCUBIC: Photon Mono, With Wash & Cure Machine 2.0)
- Coagulation Analyser (Stago: STart Max)
- Quartz Crystal Microbalance with Dissipation (Biolin Scientific: QSense)
- Add-ons (Electrochemistry, Window,Open,Humidity Modules)
- Potentiostat / Galvanostat (Gamry: Reference 600+)
- Automated Flash Chromatography System (Biotage® Selekt)
- Freeze Dryer (-105° C) Labconco: FreeZone 4.5 L
- Acid-Resistant Vacuum Concentrator Labconco: CentriVap (For 50mL Freiner Tubes and 96Well Plates)
- Microscope with Epi-LED Fluorescence Attachment: Motic: Panthera (TEC MAT BD-T)
- Spin Coater (SPS Europe: Spin200i)
- CO2 measurement cell (With control for reaction kinetics monitoring)
- Electrokinetic Analyzer for Solid Surfaces (Anton Paar: SurPASS™ 3)
- Bioindenter for Soft and Biological Samples (Anton Paar: UNHT3 Bio)
- Polarimeter VariPol C 18°C to 25°C Messröhren Bis zu 100 mm Länge

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ACHE - Analytical Chemistry for Health and Environment

Ao. Univ.-Prof. Walter Goessler

https://analytische-chemie.uni-graz.at/de/forschung/ache/

Research abstract
Research is focussed on the development and improvement of analytical methods with emphasis on inorganic analysis trough quantification of trace element (compounds) and the identification of trace element species. The developed methods are applied to answer questions and solve problems related to human health and the environment. Arsenic and the nonmetals phosphorous and sulphur play an important role in our research. Current projects focus on - identification of the arsenic compounds in hyperaccumulating mushrooms - biovolatilisation of trace elements by mushrooms - influence of elements and element compounds on bee health - trace element compounds in ultrafine particles - safe recycling of spent lithium ion Batteries

Relevant scientific infrastructure
• LC-MS/MS (Agilent Ultivo) • LC-ICPMS and LC-ICPMS/MS (UHPLC + Agilent 7900 or Agilent 8900) Alle the equipment is shared with the groups in Analytical Chemistry

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Weber Group

Ao. Univ.-Prof. Hansjörg Weber

https://www.tugraz.at/institute/orgc/research/weber-group/nmr-spectroscopy

Research abstract

Structure elucidation of small molecules by multi-nuclear NMR experiments. Analysis of kinetic data of biocatalytic conversions directly in the NMR magnet.

Relevant scientific infrastructure

- Jeol 400 MHz NMR Spectrometer
- Jeol 500 MHz NMR Spectrometer

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Bioinorganic and Coordination Chemistry

Univ.-Prof. Nadia Mösch-Zanetti

https://anorganische-chemie.uni-graz.at/de/

Research abstract
We are interested in the role of transition metals in biological systems. We research molecular processes in nature in which metals are involved. For this purpose, we develop metal complexes that replicate the active center of metalloenzymes. This not only expands our fundamental understanding but also leads to new types of catalysts. A particular focus is on the metals molybdenum and tungsten, which occur in enzymes for biological oxygen transfer reactions. Molybdenum enzymes are widely distributed in nature, are essential in key metabolic processes, and are active agents in the global biogeochemical cycles of elements such as carbon, nitrogen, and sulfur. Tungsten enzymes are much rarer so that our research provides clues as to why nature chooses tungsten as a biometal. We are also interested in manganese catalysis. Manganese is an abundant and inexpensive metal, making it an attractive option for industrial catalysis. It is also an essential trace element and is biodegradable, which is why manganese catalysts represent an environmentally friendly alternative to precious metal catalysts. We develop manganese complexes that catalyze the reduction of various substrates. Our research leads to a deep understanding of the molecular process.

Relevant scientific infrastructure
• Magnetic Susceptibility Balance MK-II • Rigaku XtaLAB Synergy-S (NAWI Graz Core Facility, located at TU Graz, usage requests from Uni Graz please use the contact given below

Address and contact data
Institute of Chemistry/Inorganic Chemistry, Uni Graz Schuberststraße 1, 8010 Graz Contact data • Name: Univ.-Prof. Nadia Mösch-Zanetti • Phone: +43 316 380 5286 • Email: nadia.moesch@uni-graz.at

Food Chemistry and Human Sensory Analysis

Assoc.Prof^{in}. Barbara Siegmund & Univ.-Prof. Erich Leitner

https://www.tugraz.at/institute/acfc/research/food-chemistry

Research abstract
The research group deals with quality aspects of food commodities (fruits, vegetables, wine, roasted products) and food contact materials (paper and cardboard, polyolefins) with a focus on (i) odour and off-odour of products, and (ii) the presence of compounds of toxicological concern. To cover this, analytical chemistry mainly based on separation sciences due to the usual complexity of the samples is used on the one hand. On the other hand, specific techniques are applied to identify and characterise the flavour quality. Projects are dealing with – Characterization and safety evaluation of (recycled) food contact material – Method development for the quantification of compounds of toxicological concern – Method development for the identification and quantification of odour active compounds – Identification of flavour formation pathways (bioflavour formation as well as thermal flavour generation) in mainly plant material – Identification of off-flavour compounds and development of strategies for off-flavour prevention in food and food contact material – Correlation of flavour compounds with neoformed contaminants; development of mitigation strategies – Characterisation of the sensory product characteristics using up-to-date sensory methods

Relevant scientific infrastructure
• Several GC systems with conventional detectors (FID, BID, NPD, ECD) • GC-MS with quadrupole and time of flight mass filters • Comprehensive GCxGC-MS • Comprehensive GCxGC-SCD-FID for sulfur selective detection • Automated sample preparation based on headspace techniques (SPME, arrows, vacuum ITEX, Linex, mono trap) • Microwaved based sample preparation with autosampler • Microwaved based moisture analyzer • Gas chromatography olfactometry (GC-O/FID, GC-O/MS) • Sensory laboratory equipped according to standards • A specifically trained sensory test panel and a consumer panel ad hand • Vast collection of odour active compounds (approx. 2.000 pure compounds and extracts) • In-house retention index database specifically designed for the identification of odour active compounds

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Inorganic Chemistry Groups

Univ.-Prof. Frank Uhlig (head of the institute), Assoc.-Prof. Michaela Flock (vice head of the institute), Assoc.-Prof. Roland Fischer (vice head of the institute)

https://www.tugraz.at/institute/ac/home

Research abstract

The Institute of Inorganic Chemistry deals with molecular, analytical and material aspects of the main group elements with a strong emphasis on organometallic compounds including theoretical calculations. The institute consists of two major branches

- Synthesis and Materials
- Analytics and Materials

and is divided into six larger working groups

- working group Univ.-Prof. Frank Uhlig
- working group Assoc.-Prof. Michaela Flock
- working group Assoc.-Prof. Roland Fischer
- working group Ao. Univ.-Prof. Christoph Marschner
- working group Assoc.-Prof. Heinz Amenitsch
- working group Priv.-Doz. Michael Haas

While the major facilities of the institute are located in Graz, the institute is unique by also having an outstation at the synchrotron ELETTRA in Trieste (Italy) running the AustroSAXS beamline on behalf of the Austrian science community.

Besides fundamental research activities, the working groups of the institute are involved also into applied research projects covering sometimes the whole range of inorganic chemistry including analytical problems. As one of the latest examples for applied basic research projects the CD Laboratory “Novel Semiconductor Materials based on functionalized Hydrosilanes” (head of research unit: M. Haas; Duration: 2024-2031) can be mentioned.

Relevant scientific infrastructure

- AustroSAXS Beamline (synchrotron ELETTRA, Trieste); https://www.elettra.eu/elettra-beamlines/saxs.html
- DXRL Beamline (synchrotron ELETTRA, Trieste); https://www.elettra.eu/elettra-beamlines/dxrl.html
- **S**oft **Ma**tter **Ap**plication Lab; joined project between TU Graz – Anton Paar (– Uni Graz) https://www.tugraz.at/en/institutes/ac/equipment-services/somapp-lab
- Elemental Analysis Service as NAWI Graz Core Facility; https://www.tugraz.at/en/institutes/ac/equipment-services/equipment-graz/elemental-analysis
- Single Crystal X-ray Diffraction as NAWI Graz Core Facility; https://www.tugraz.at/en/institutes/ac/equipment-services/equipment-graz/x-ray-diffraction
- QUAD Systems 400 MHz NMR system dedicated to hetero nuclei determination; https://quadsystems.tech/consoles/
- 3 Bench Top NMR devices NMReady60 from Nanalysis; https://www.tugraz.at/en/institutes/ac/equipment-services/equipment-graz/benchtop-nmr

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Enabling Technologies

Univ.-Prof. C. Oliver Kappe

http://goflow.at

Research abstract
For the past decade the focus of the Kappe laboratory has been directed towards flow chemistry/microreaction technology, encompassing a wide variety of synthetic transformations and experimental techniques. Notably, these include handling hazardous, toxic and/or unstable reagents and gases in flow environments, many times in extreme temperature and pressure regimes reaching the near- or supercritical state. Flow processing has been executed both in monophasic or multiphasic (i.e., liquid/liquid, solid/liquid, gas/liquid, gas/liquid/solid) flow regimes using a range of reactor designs, and utilizing membrane separation techniques, particularly towards the multistep synthesis of APIs. The group additionally has experience in PAT, machine learning/AI, and flow photochemistry/electrochemistry applications. A particular focus is directed towards sustainable technologies, i.e. using water as reaction medium.

Relevant scientific infrastructure
Our laboratories occupy ca. 400 m2 of well-equipped state-of-the-art laboratory space at the Institute of Chemistry (IfC) at the University of Graz. The group is well-equipped with all standard analytical instrumentation for performing organic synthesis (HPLC-UV(DAD), LC-MS(ESI), GC-FID, GC-MS(EI), semi-preparative HPLC-UV, automated flash chromatography, etc.). • Specific Flow reactors and analytical instrumentation: http://goflow.at/technology-overview/

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Environmental Metallomics

Ao. Univ.-Prof. Doris Kuehnelt & Assoz. Prof. Georg Raber

https://analytische-chemie.uni-graz.at/de/forschung/em/

Research abstract
The research focus of our working group is Metallomics, which addresses the distribution, dynamics, function, and significance of metal and metalloid species in biological systems and investigates their profiles in the environment, in food sources and in living organisms. We particularly focus on trace elements (mainly arsenic and selenium, but also others) with emphasis on the profiles of trace element species in biological, environmental and human samples (blood, urine). We correlate these with health aspects and investigate the biotransformation/detoxification of element species in organisms and ecosystems. Besides our research activities in the field of trace element speciation analysis we are capable of determining organic compounds (metabolic products, toxicants etc.) by GC triple quadrupole MS, HPLC coupled to ESI triple quadrupole MS or high resolution ESI Orbitrap MS, as well as total trace element contents in various sample matrices.

Relevant scientific infrastructure
• Microwave-assisted acid digestion systems (EMLS Ultraclave 4 and ETHOS) • Various HPLC systems (Agilent 1100, 1260; Thermo Ultimate 3000) • Agilent 7900 ICPMS • Agilent 8800 ICP-QQQ-MS • Agilent 7890A GC with Agilent 7000 Triple Quad MS • Agilent Agilent 6460 Triple Quad LC-MS • Thermo QExactive ESI-Orbitrap-MS

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Quantum Chemistry

Univ.-Prof. A. Daniel Boese

https://quantchem.at

Research abstract

• Theoretical Chemistry: Method Development:
  ○ Embedding Methods (both molecular/periodic)
  ○ Density Functional Theory
  ○ Analysis of Intermolecular Interactions
  ○ High-Accuracy/Extrapolation
 	
• Computational Chemistry: Method Application:
  ○ Molecular Crystals
  ○ Reaction Path Analysis
  ○ Solid-State Reactions
  ○ Infrared Spectra
  ○ Crystal Structure Prediction (CSP)

Relevant scientific infrastructure
• High-Performance (HPC) Computer Cluster- approximately 1000 Cores of the AG Quantum Chemistry • HPC Computer Cluster of the University of Graz (GSC)- approximately 3000 Cores • HPC Computer Cluster at Vienna (Vienna Scientific Cluster)

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Functional Ceramics

Assoc.Prof. Jurij Koruza, Ao. Univ.-Prof. Klaus Reichmann

https://www.tugraz.at/institute/ictm/research/koruza-group

Research abstract

High-performance electroceramics are becoming increasingly important parts of current and emerging technologies in the fields of consumer electronics, data storage, autonomous vehicles, automotive industry, sensors and power generators for the Internet of Things, as well as medical robotics and in-body sensors. Our group is focused on material development, processing, microstructure design, and characterization of sustainable advanced electroceramics. Examples include **piezoelectrics**, (anti)**ferroelectrics**, **dielectrics**, **multiferroics**, and **thermistors**.

We investigate the structure-microstructure-property relationships of electroceramic materials and we are specialized in **ceramic processing** using conventional and advanced techniques. The latter include environmentally-friendly low-temperature processing and additive manufacturing of ceramics.

Our group utilizes a wide range of **methods for structural/microstructural analysis**, **processing control**, and characterization of **functional electrical properties**. To get a deeper insight into material´s mechanisms, we are also developing new in situ measurement methodologies combining electromechanical and structural analysis techniques, for example X-ray or neutron diffraction.

Relevant scientific infrastructure

Ceramic processing equipment

- Chemical laboratories for ceramic processing
- High-energy ball milling, powder particle size characterization (dynamic light scattering)
- High-temperature furnaces with atmosphere control (up to 1700 °C)
- Powder forming equipment (uniaxial and isostatic pressing tools)

Characterization methods for ceramics

- Ceramographic sample preparation (diamond cutting, grinding, polishing)
- X-ray diffractometers
- High-resolution digital optical microscopy
- Thermal analysis (thermogravimetry, differential scanning calorimetry, mass spectroscopy, dilatometry)

Electrical and electromechanical measurements

- Dielectric measurements over a broad temperature and frequency range
- High-voltage (20 kV) polarization and strain measurements (ferroelectric hysteresis loops)
- Determination of piezoelectric coefficients
- Laboratory for piezoelectric resonance (small- and large-signal resonance measurements using dielectric spectroscopy and laser vibrometer).
- Custom-made electrical fatigue and lifetime testing

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Medicinal Organic Chemistry

Assoz. Prof. Toma Glasnov

https://chemie.uni-graz.at/de/forschen/organische-bioorganische-chemie/

Research abstract
Efficient synthesis of biologically active small molecules via traditional/modern methods. The main focus is on organic synthesis and development of mediators for ion channels in human cells. The new substances serve as light-sensitive “on-off-switches” for the research and development of new cancer therapies in a close cooperation with the MedUni-Graz and JKUni Linz.

Relevant scientific infrastructure
• General lab instrumentation – HPLC, LC-MS, UV-Vis, Microwave etc.

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Wilkening Group

Univ.-Prof. H. Martin R. Wilkening

https://www.tugraz.at/institute/ictm/research/wilkening-group/

Research abstract

Ion Dynamics in Solids. The Wilkening group focuses on preparing, characterizing, and functionalizing new materials for modern energy storage systems. Emphasis is put on spectroscopic studies shedding light on micro- and macroscopic ionic transport processes in crystalline, nanostructured, and amorphous or glassy solids. In particular, we use solid-state nuclear magnetic resonance (NMR) and broadband conductivity spectroscopy (impedance data) to investigate short- and long-range ion dynamics in a variety of functional materials that are relevant for, e.g., energy storage applications.

Phenomena include the study of dimensionality effects, nano-size effects, interfacial ion transport and the influence of structural disorder on self-diffusion. Recently, we also studied the coupling of translational with rotational dynamics in a range of functional materials.

Keywords: energy/battery materials, solid-state diffusion, ion dynamics (Li, Na, F ion conductors), amorphous and nanocrystalline solids, nanoglasses, insertion materials, NMR spectroscopy (relaxation experiments, stimulated echo correlation spectroscopy (SAE)), impedance/conductivity spectroscopy, solid-state electrochemistry (CV, GCPL, polarisation measurements), mechanochemistry, non-equilibrium phases

Recent examples:

A. Jodlbauer, K. Hogrefe, B. Gadermaier, H. M. R. Wilkening, Small Sci. (2024), 2400199 Link
T. Scheiber, B. Gadermaier, M. Finsgar, H. M. R. Wilkening, Adv. Funct. Mater. (2024) 2404562. Link
L. Schweiger, K. Hogrefe, B. Gadermaier, J. L. M. Rupp, H. M. R. Wilkening, J. Am. Chem. Soc. 144 (2022) 9597 Link

Relevant scientific infrastructure

High-resolution and time-domain solid-state NMR:

- Bruker 500 MHz solid-state spectrometer (Avance III), 1.3-mm and 2.5-mm MAS probes (up to 60 kHz spinning speeds; 1D and 2D NMR experiments for ^{1}H, ^{19}F, ^{31}P, ^{29}Si, ^{13}C, ^{27}Al, ^{23}Na etc.
- Bruker 300 MHz solid-state NMR spectrometer for dynamic measurements down to 8 K, several static NMR probes to measure variable-temperature relaxation rates in the laboratory and rotating frame of reference

Electrical measurements:

- Several (fully automated) conductivity spectrometers (Novocontrol, down to 10^{-12} S/cm, 1 µHz . 3 GHz, -150 °C . 800 °C) for impedance and dielectric measurements
- Solid-state electrochemistry: several potentiostats and galvanostats for all kinds of battery tests (BioLogic, Parstat - operated in combination with climate chambers)

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BioNMR

Ao. Univ.-Prof. Klaus Zangger

https://nmr.uni-graz.at

Research abstract
In the BioNMR group we use high-resolution NMR (nuclear magnetic resonance) spectroscopy for the determination of structural and dynamical details of both small organic and biomolecules. Some recent main targets include proteins involved in the toxicity of bacterial pathogens and their interactions with DNA. Other work has centered on the investigation of enzymatic mechanisms of membrane-bound proteins, for example yeast V-ATPase. We have also used NMR spectroscopy to investigate the interactions of intrinsically disordered proteins involved in the generation of Alzheimer's disease. An important aspect of our research is the development of novel NMR techniques. We have developed several approaches to enhance the resolution of NMR spectra by pure shift techniques (modulation of the size of scalar coupling) and an NMR approach which is based on the use of paragmagnetic relaxations enhancements to provide additional structural information for protein studies and to determine the location of membrane-bound peptides in micelles and other membrane-mimetics.

Relevant scientific infrastructure
• Bruker Avance III 300 MHz NMR spectrometer (part of the Uni Graz NMR core facility • Bruker Avance Neo 500 MHz NMR spectrometer (part of the Uni Graz NMR core facility • Bruker Avance III 700 MHz NMR spectrometer (part of the Uni Graz NMR core facility

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Working Group Gollas

Assoc.Prof. Bernhard Gollas

https://www.tugraz.at/institute/ictm/research/gollas-group/

Research abstract

The Gollas Group is interested in charge transfer reactions at solid/liquid interfaces. Research activities extend from fundamental studies of electrode reactions to the electrodeposition of novel materials and applications in the fields of industrial electroplating and electrochemical energy storage and conversion. All classical electroanalytical methods are used including electrochemical impedance spectroscopy, rotating disc, rotating cylinder and rotating ring-disc electrode as well as ultramicroelectrode techniques. They are combined with structure-sensitive methods (spectroscopy, microscopy, diffraction, scattering, tomography) ex-situ and, if necessary and feasible, in-situ or in-operando.

Relevant scientific infrastructure

- Potentiostat/Galvanostat BioLogic VMP-300, 6-Channel (1 Impedance)
- Potentiostat/Galvanostat Autolab 302N, with Bipotentiostat-, Impedance-, Analog-, Low-current-, Fast-scan-, Analogfilter and Integrator-Modules
- Potentiostat/Galvanostat Autolab 128, with pH/pX-Module
- Potentiostat/Galvanostat Autolab 100
- Rotating disk-/Ring-disk-electrode Pine Research Instrumentation
- Rotating cylinder Hull-cell Autolab
- BaSyTec CTS-LAB-XL Battery test system, 8-Channel
- Test rig for redox-flow batteries
- Pulse- and Pulse-Reverse Power Source up to 150 A
- GS Glovebox ALPHA 2 with Ar atmosphere equipped with solvent absorber and refrigerator

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Carraro Group

Ass.-Prof. Francesco Carraro

https://www.tugraz.at/institute/ptc/research/carraro-francesco

Research abstract
The Carraro group works on the synthesis, characterization and application of porous materials, with a particular focus on Hydrogen-bonded Organic Frameworks (HOFs) and HOF-based composite materials and the use of in situ characterization techniques.

Relevant scientific infrastructure

The AG Carraro is working at the Institute of Physical and Theoretical Chemistry and have access to the equipment of the Institute. The most relevant equipment is:

- X-ray Diffractometer, Rigaku SmartLab, 9 kW rotating Cu anode, measurement in Bragg-Brentano, transmission, grazing incidence and in-plane geometry are possible.
- Raman Microscope, Thermo Scientific™ DXR™ 2, equipped with two lasers (532 and 785 nm), several objectives and a motorized stage, acquisition of single point spectra, chemical maps and in situ and time-resolved studies are possible.

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Single-Molecule Chemistry

Univ.-Prof. Leonhard Grill

https://nano-lab.uni-graz.at

Research abstract

The Single-Molecule Chemistry group uses scanning tunnelling microscopy/spectroscopy and atomic force microscopy to study and **selectively manipulate single molecules on surfaces**. Manipulation is performed by light of specific wavelength or with the STM tip, using chemical forces, tunnelling electrons or the electric field. Such manipulation experiments make it possible to **selectively trigger chemical reactions, investigate molecular functions or displace individual molecules, atoms or nanostructures with atomic precision**. Our interests range from chemical processes of single atoms and molecules to the bottom-up growth of two-dimensional supra- and macromolecular assemblies. Our research includes **various kinds of functional molecules with mechanical, chemical, electronic, optical or electrical functionalities**.

Main research topics:

- Triggering and understanding *bond formation and dissociation reactions* at the single molecule level
- *Bottom-up construction of molecular nanostructures*: supramolecular growth and on-surface polymerization, in which molecular building blocks are connected to construct pre-defined, stable networks on surfaces
- *Growth of two-dimensional materials* as for instance graphene
- *Molecular switches*: the mechanism of single-molecule switches, based on intramolecular isomerization or proton transfer, is studied and a strong influence of the immediate environment on each molecule – even for single atoms in the vicinity of the molecule – has been found
- *Catalytic processes* where the metal surface acts as heterogeneous catalyst for adsorbate reactions; using different surfaces, the actives sites of molecular activation could be precisely identified
- *Single-molecule motion*: our group has demonstrated the first rolling molecular wheel across a surface and could also displace individual molecules over relatively large distances with extremely high precision – even allowing direct measurement of the speed of a single molecule
- *Molecular wires* that consist of only a single polymer strand: by pulling individual polymers off of a surface with the tip of the scanning tunnelling microscope, we were able to measure for the first time the conductivity of individual molecular wires as a function of their length and to characterize molecular knots
- *Nanomachines with molecular motors*: these molecules either contain the motor in their chemical structure or gain this function as 'adsorbate motors' by combining a molecule with a surface where they can move unidirectionally with 100% efficiency, and even transport individual carbon monoxide molecules as "cargo"

Relevant scientific infrastructure

- Scanning tunnelling microscopes (STM) and atomic force microscopes (AFM) working under ultrahigh vacuum and at temperatures between 4 K and 400 K
- Scanning tunnelling microscopes (STM) in ambient conditions at the solid-air interface
- Scanning tunnelling microscope (STM) in ambient conditions at the solid-liquid interface
- Low energy electron diffraction (LEED)
- Molecular deposition techniques: Knudsen cells, Si wafer, electrospray injection, pulsed valve
- X-ray photoelectron spectroscopy (XPS) under ultrahigh vacuum with a mono-chromated x-ray source
- Various light sources in the UV and visible range, including a femtosecond laser for two-photon photoemission spectroscopy and time-resolved STM studies

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Sustainable Catalysis

Univ.-Prof. Katalin Barta Weissert

http://bartagroup.org/

Research abstract

The research program within the working group broadly addresses scientific challenges that help to transition from a linear, fossil-dependent industry, to a one based on renewable resources. To this end, we develop methods that are able to integrate widely available sustainable carbonaceous material streams (such as renewable biomass, plastic waste) into the circular bioeconomy.

While deeply rooted in sustainable catalysis and green chemistry, the research group follows a highly interdisciplinary approach. Research areas related to emerging biorefinery concepts, circular bioproducts, materials and polymers, homogeneous and heterogeneous catalysis, chemical engineering and organic chemistry are represented and integrated. Accordingly, the research group features PhD students and post-docs with a wide range of backgrounds and skills, and the regular group meetings address a variety of research topics.

Relevant scientific infrastructure

- AGILENT TECHNOLOGIES 6230 HPLC-ToF-MS-UV/IR system [NAWI Graz Core Facility]
- AGILENT TECHNOLOGIES 8890/5977B DUAL FID/ Mass spectrometer system
- AGILENT TECHNOLOGIES 5975c Mass spectrometer
- BÜCHI Minipilot glass reactor (15L volume, split reflux/distillation head, sampling unit)
- KRUESS K100C Force tensiometer
- KRUESS BP100 Bubble tensiometer
- MBRAUN Unilab plus Glovebox
- MBRAUN MBSPS5 Solvent purification system
- MODERN WATERS Microtrox acute toxicity analyser
- NETZSCH 204 F1 Dynamic scanning calorimeter
- NETZSCH 449 FF Simultaneous thermal analyser
- NETZSCH 204 F1 Dynamic mechanical analyser
- PARR INSTRUMENTS 4575 High temperature/high pressure reactor (0.5L, Hastelloy C) [Central lab]
- PARR INSTRUMENTS Various autoclaves (50 mL – 1000 mL, Hassteloy C or stainless steel)
- RADLEYS Reaction stations in various sizes (2x Carousel (12x 20 mL), 1x Tornado (6x 250 mL)
- SHIMADZU NEXERA HPLC-UV system
- THERMO SCIENTIFIC ISQ 7610 Mass spectrometer system
- THERMO SCIENTIFIC GC240 Orbitrap Exploris

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Biocatalytic Synthesis

Univ.-Prof. Wolfgang Kroutil

https://biocatalysis.uni-graz.at/

Research abstract

The research focuses on cutting-short organic synthetic (asymmetric) routes to various types of molecules needed as pharmaceuticals, aroma compounds, vitamins and polymer buildings blocks by employing biocatalysts. We perform basic research to develop novel bio-based methods for (asymmetric) reactions being inspired by natures catalyst, the enzymes. We contribute to a sustainable future by designing highly selective transformations which can be performed in general in water/buffer thereby minimizing waste and the catalysts are made from renewables and are biodegradable. Significant effort is dedicated to substitute existing routes to pharmaceuticals and agrochemicals by shorter, less expensive ones to ensure the position of Europe as an international producer.

As an interdisciplinary group we use methods from organic chemistry, biotechnology, biochemistry, structural biology and molecular biology.

Relevant scientific infrastructure

- High-Throughput Robotic Screening Platform including 2 robotic arms (1x 96 tips, 1x 8 tips), incubator, multiwell-plate reader, colony picking, centrifuge
- Glove box for biocatalysis (using water as solvent)
- nanoDSF, polarimeter
- Various GC-FIDs, HPLC-DADs, GC-MS, HPLC-MS
- Speedvac, Multi-Well plate reader, UV-VIS spectrophotometer, etc.

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Advanced X-ray Scattering

Ass.-Prof. Stefan Kowarik

https://chemie.uni-graz.at/en/kowarik-lab/

Research abstract
Our work is focused on advanced x-ray scattering methods for surface analysis, optical analytics as well as artificial neural networks that facilitate analysis and interpretation of the large amounts of data generated by these methods. We study deposition processes (vacuum deposition, spin coating) of mainly organic thin films with in situ X-ray experiments that do not only uncover the final structure but also transient structures that would be missed otherwise. Examples of our work include molecular switches at surfaces and optical patterning of molecular films during deposition.

Relevant scientific infrastructure

- PANalytical Empyrean Powder diffractometer with Mo (hard X-ray) tube
- Surface diffraction with microfocus Cu tube and heavy load diffractometer for in situ setups
- Regular user of synchrotron X-ray facilities (ESRF, DESY, BESSY, Diamond, SLS) – I am happy to help with proposals or to cooperate

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Slugovc Group

Assoc.Prof. Christian Slugovc

https://www.tugraz.at/institute/ictm/research/slugovc-group

Research abstract
Research in the Slugovc Group focuses on the advancement of catalytic polymerization reactions by targeting more efficient catalytic processes and by developing a comprehensive mechanistic understanding of the studied reactions at the molecular level. The first research focus is on olefin metathesis-based reactions such as Ring Opening Metathesis Polymerization (ROMP) or cross-metathesis based process like Acyclic Diene Metathesis (ADMET). Amongst initiator/catalyst development also new materials based on olefin metathesis routs are researched. In particular porous polymers prepared with olefin metathesis polymerization are developed. A second field of competence encloses proton transfer based polyaddition reactions in their anionic variant, e.g. aza-, thia- and oxa-Michael reactions as well as epoxy, cyclic carbonate and isocyanate-based resins. For these reactions, organocatalytic ways to accelerate and to increase the substrate scope are developed and materials based on the novel ways of catalyzing the reactions are investigated. In this context, covalent adaptable materials are in the focus of the research work.

Relevant scientific infrastructure
• Perkin Elmer DSC6000 - Modulated temperature differential scanning calorimeter (Temperature range -40 to 400°C)

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Breinbauer Group

Univ.-Prof. Rolf Breinbauer

https://www.tugraz.at/institute/orgc/home

Research abstract

Rolf Breinbauer's research group is interested in 1) the development of tool compounds for Chemical Biology and 2) the development of new synthetic methods for Organic Chemistry. The first program ranges from molecular probes to investigate the biosynthesis of natural products and understanding its enzymology, over the development of probes for activity-based protein profiling (ABPP), to the design and synthesis of inhibitors of enzymes. The Breinbauer group focuses on targets which have not been investigated by chemical means so far. A notable achievement is the development of Atglistatin® and NG-497 the first inhibitors of murine resp. human ATGL (adipose triglyzeride lipase), with which ATGL could be validated as a drug target. The second programme involves transition metal catalysed reactions and the development of new biocatalytic methods involving gene reductases.

Relevant scientific infrastructure

- Instrument GC-MS: Agilent Technologies 7890A GC + 5975C mass selective EI detector
- Instrument HPLC-MS: Agilent Technologies 1200 Series HPLC + 6120 Quadrupole LC/MS
- Instrument HPLC-MS: Shimadzu LCMS-2020
- Instrument Semipreparative RP-HPLC-MS: Thermo Scientific UltiMate 3000 system

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