# CHEMISTRY DEPARTMENT UNIVERSITY OF FRIBOURG

ACTIVITY REPORT 2022 - 2023



UNIVERSITÉ DE FRIBOURG UNIVERSITÄT FREIBURG

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### WELCOME

# From the President Transformative Research & Education

Chemistry is playing an increasingly important role in modern society. Aware of the importance of this discipline in technology, we strive to create an international environment where, through research and teaching, both undergraduate and graduate students acquire not just the scientific knowledge, but also the skills that will help them to adapt to an ever-changing word. We hope to instill in them the passion for learning, which will last throughout their career, to teach them the importance of teamwork and foster their spirit of innovation and creativity.

In the last two years, the successful hire at a junior level strengthened our research capabilities in theoretical chemistry with potential applications in machine learning and artificial intelligence. The research activity of our department is characterized by high interdisciplinarity, highly stimulating research environment, top-level research infrastructure and excellent working conditions. The faculty, with the help of brilliant students from all over the word, seeks to solve problems of high fundamental and practical importance and promote a culture of innovation and collaboration. Nanotechnology, food science, polymer, organic and inorganic chemistry applied to novel drug synthesis, materials for energy storage applications are only some of the exciting research topics investigated in the department. We have also made significant infrastructure upgrades to support our research, including the installation of SAXSPoint 5.0 with MetalJet X-ray source, the first of its kind in Switzerland. In terms of teaching, we also recently established a virtual reality classroom for chemistry education, our efforts to adapt our curriculum to this new technology is ongoing. Taken all together, the chemistry department is ready for the future, will continue to increase the quality of research and teaching. In the coming years, we will continue to adopt new strategies and technologies to further improve our teaching and research activities. Finally, I would like to thank all the members of our department for their strong

commitment and support!

President of the Department of Chemistry Prof. Dr. Ali Coskun

Ali Coshyn

The grand challenges of the 21st century are waiting for the next generation scientist - you! Join us to discover the wonders of chemistry! **Department Head** 

## Prof. Ali Coskun



Chemistry is like family. It is all about bonding together.



### ORGANIC PHOTOCHEMISTRY

## **Using light to create new substances**

Organic synthesis is the science dedicated to the preparation of carbon-based substances in the laboratory. Photochemistry is the science studying how light can transform matter. Thus, organic photochemistry uses light to create new molecules.

## Prof. Christian BOCHET

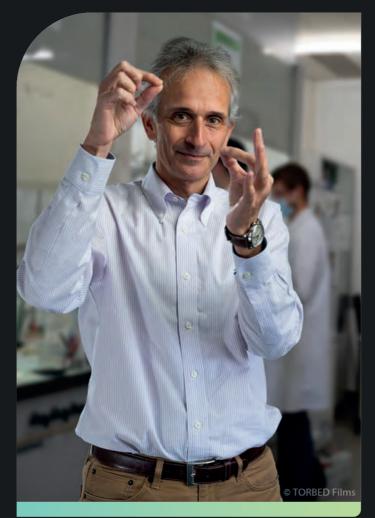
Our group's aim is to use light as a safe, inexpensive and environmentally friendly alternative to classical chemical reagents. To be able to reach this long-term goal, we approached the problem from two different sides at the same time: a) finding new reactions promoted by light, giving new substances that are tested for their pharmaceutical properties and optimising existing reactions by replacing certain components by light, in collaboration with the chemical industry. b) trying to understand the fundamentals of photochemistry, by designing model reactions to test the currently used hypotheses, and studying them both experimentally and by computer-assisted modelling.

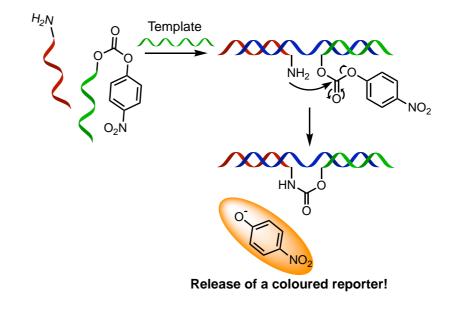
The future of chemistry is bright

In parallel to these studies, we are also interested in the development of new techniques to detect and identify short DNA and RNA fragments. We have successfully prepared a very fast sensor for such fragments, that is now being tested for the identification of pathogens, such as Listeria or other bacterial strains.

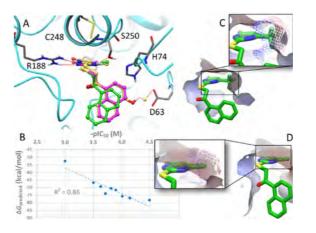
Finally, our group has a long-time collaboration with the University of Yaoundé, Cameroon, for the isolation of pharmaceutically active substances from local plants. Starting from raw extracts, several new substances were found, some of them with promising therapeutic effects.

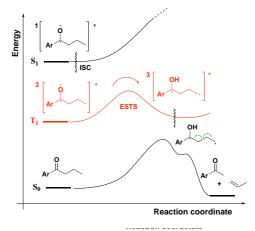
With the rarefaction of many raw materials, it is increasingly important to be able to use light, the only energy source reaching our planet, in all possible types of applications. After all, Nature is able to produce very large molecules with incredible precision by just combining carbon dioxide and water with the help of light. The future of chemistry is linked to the ability of scientist to do just the same!





DNA-templated synthesis: how to use DNA to accelerate chemical reactions





BOCHET

### Group



#### **Recent publications:**

Influence of Chlorinating Agents on the Formation of Stable Biomarkers in Hair for the Retrospective Verification of Exposure Severin V. Martz, Matthias Wittwer, Chia-Wei Tan-Lin, Christian G. Bochet, Maximilian Brackmann, and Christophe Curt, Anal.Chem, 2022, 94, 16579–16586.

**3,3',5,5'-Tetramethoxybenzoin: a forgotten photolabile protecting group** Dario Bragagnolol and Christian G. Bochet, Photochemical & Photobiological Sciences, 2022

#### Development and Scale-Up of a Novel Photochemical C-N Oxidative Coupling

Alan Robinson, Michael Dieckmann, Jean-Philippe Krieger, Thomas Vent-Schmidt, Dominique Marantelli, Ralf Kohlbrenner, Denis Gribkov, Levente L. Simon, David Austrup, Alexandre Rod, and Christian G. Bochet, Org. Process Res. Dev. 2021, 25, 2205–2220

WEBSITE: https://thebochetgroup.wordpress.com/

Medicinal chemistry: finding improved enzyme inhibitors

Photochemistry: understanding how light promotes chemical reactions

### LABORATORY OF FUNCTIONAL MATERIALS

# Exploring new materials approaches for energy and environmental challenges

## Prof. Ali COSKUN

Renewable Energy for a better tomorrow CO<sub>2</sub> emissions into the atmosphere account for the majority of environmental challenges and its global impact in the form of climate change is well-documented. Accordingly, the development of new, sustainable materials approaches to capture and convert CO<sub>2</sub> into value-added products is essential. Whereas the increased availability of renewable energy is curbing our reliance on fossil fuels and decreasing CO<sub>2</sub> emissions, the widespread adaptation of renewable energy still requires the development of high energy density batteries i.e., lithium ion batteries (LIBs). In this direction, our research program targets the sustainable development of functional materials by creating family of porous organic polymers, membranes, electrolytes and supramolecular polymers to solve critical energy and environmental problems with a particular emphasis on high energy density Li-ion batteries, gas capture&separation and catalysis applications. The focus of our research is to identify fundamental design principles in these materials in order to correlate the functions at the molecular level to the resulting materials properties.

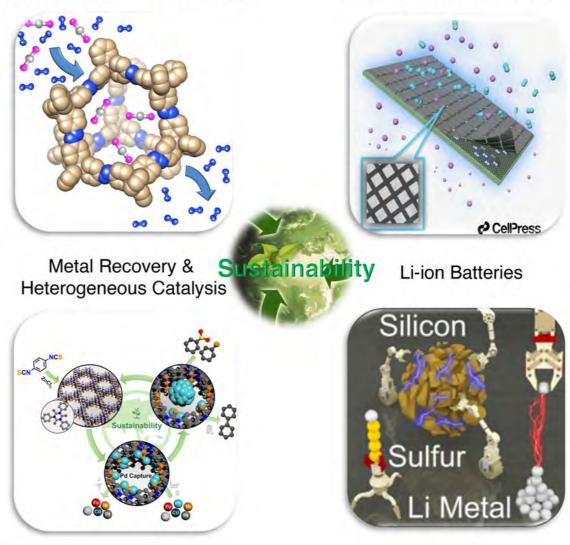
Our group has been developing porous organic polymers (POPs) with precise control over their porosity and surface chemistry for  $CO_2$  capture, separation and conversion. To realize simultaneous  $CO_2$  separation and conversion, we are also developing catalytically active two-dimensional membranes and POPs. More recently, we also expanded our research efforts to cover atmospheric water capture and recovery of precious metals from waste water conditions.

In particular, the latter appoach targets to achieve circular chemistry by recycling various metals for reuse. In the area of LIBs, we have recognized the potential of supramolecular chemistry as a general strategy for solving the capacity-fading problem associated with high energy density electrode materials such as Li-metal, silicon and sulfur, which offer extremely high battery capacity compared to conventional LIBs. Recently, we also expanded our research efforts towards the development of liquid and solid-state electrolytes. Accordingly, we have demonstrated how molecular-level design can be directly translated into an improved electrochemical performance in high energy density LIBs.

These research directions provide an outstanding opportunity to my students to develop their skills in polymer, materials and electro- chemistry, enhanced by the experience of collaborating with scientists from other disciplines.



### CO<sub>2</sub> Separation and Conversion



Overview of research activities in the Coskun Research Group ranging from CO<sub>2</sub> capture, storage conversion to gas separation membranes to high energy density Li ion batteries.

### Gas Separation Membranes

## COSKUN

### Group



#### Selected publications:

Electrolyte engineering for highly inorganic solid electrolyte interphase in high-performance lithium metal batteries Zhao, Y.; Zhou, T.; Jeurgens, L. P. H.; Kong, X.; Choi, J. W.\*; Coskun, A.\* Chem, 2023, 9, 682-697.

### Fast Light-switchable Polymeric Carbon Nitride Membranes for Tunable Gas Separation

Ashirov, T.; Siena, J. S.; Zhang, M.; Yazaydin, A. O.; Antonietti, M.\*; Coskun, A.\*, Nat. Commun., 2022, 13, 7299.

#### Porous Polyisothiocyanurates for Selective Palladium Recovery and Heterogeneous Catalysis

Song, K. S.; Ashirov, T.; Talapaneni, S. N.; Clark, A. H.; Yakimov, A.; Nachtegaal, M.; Copéret, C.; Coskun, A.\*, Chem, 2022, 8, 2043-2059.

WEBSITE: http://www.coskunlab.com/

### BIONANOMATERIALS

## Using nanoparticles to influence cells and cell mechanics

## Prof. Alke FINK

There is a lot of stuff you can do with nanoparticles Cellular behaviour is strongly dependent on the mechanical response of the substrate which has been shown to regulate important functions such as adhesion, migration and differentiation. The possibility to selectively control and direct cellular functions through materials selection, design and processing has huge value for e.g. improving patient health.

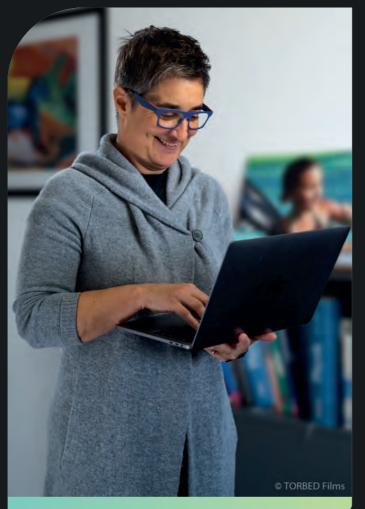
(Nano)particle surfaces offer a unique platform to study the interplay between cells and their physical environment.

The adsorption of particles to surfaces introduces novel contextual cues which can potentially alter particle and surface biorecognition with consequences for cell mechanics.

In the last year and to understand how particle adsorption alters and defines nanobiointeractions, different bioactive particle surfaces were produced through electrostatically- mediated assembly. In general, we observe that under specific conditions, cells can remove these adsorbed particles in a manner akin to that of the famous robotic vacuum cleaner.

To highlight the contribution of mechanical properties to the capacity for cellmediated clearance, poly(N-isopropylacrylamide) particles with differing stiffness were used to fabricate surfaces. Macrophages cultured on these particle surfaces showed a preference for stiffer particles. Particle recognition was noted to occur through reorganisation of adhesion complex proteins such as vinculin. More complex particle bearing substrates are currently under investigation to examine the contribution of hierarchical topography to surface particle clearance. This work is funded through the NCCR for BioInspired Materials (51NF40-182881). All work is done in collaboration with my co-chair Prof. Barbara Rothen-Rutishauser and the Adolphe Merkle Institute (AMI) at the University of Fribourg.

Other main topics of the group evolve generally around engineered nanoparticles and include e.g. (1) the development of analytical methods to detect and quantify nanoparticles in complex media (such as consumer products, physiological fluids etc.), (2) nanoparticle dosimetry and (3) nanoplastics etc.



## Fink

### Group



Prof. Fink currently has two affiliations, one in the Chemistry Department and the other one at the Adolphe Merkle Institute, where she co-chairs the BioNanomaterials group with Prof. Rothen-Rutishauser.

#### ecent publications:

The Influence of Liquid Menisci on Nanoparticle Dosimetry in Submerged Cells

Christina Glaubitz, Laetitia Haeni, Eva Sušnik, Barbara Rothen-Rutishauser, Sandor Balog, Alke Petri-Fink; Small (2023)

The need for awareness and action in managing nanowaste Fabienne Schwab, Barbara Rothen-Rutishauser, Aline Scherz, Thierry Meyer, Bedia Begüm Karakoçak, Alke Petri-Fink; Nature Nanotechnology (2023)

Correlative Light, Electron Microscopy and Raman Spectroscopy Workflow To Detect and Observe Microplastic Interactions with Whole Jellyfish

Jessica Caldwell, Céline Loussert-Fonta, Gaëlle Toullec, Niclas Heidelberg Lyndby, Beat Haenni, Patricia Taladriz-Blanco, Begoña Espiña, Barbara Rothen-Rutishauser, Alke Petri-Fink; Environmental Science & Technology (2023)

WEBSITE: https://www.ami.swiss/bionanomaterials/en/

Image representing the above-described research: Cells can act like vacuum cleaners and can remove particle carpets

### **BIOINORGANIC AND COORDINATION CHEMISTRY**

## Antimicrobial metal ions and new devices

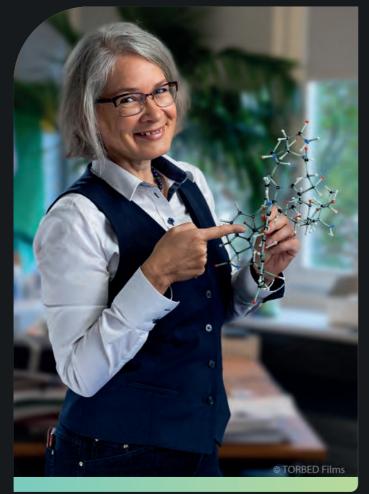
Prof. Katharina FROMM

The periodic table is a vast playground With the emergence of multi-resistant bacteria which are impossible to combat with standard antibiotics, the interest in antimicrobial metal ions has increased over the past years. Little is known about how certain metal ions interact with biomolecules such as proteins, DNA or sugars. We are thus interested in learning how antimicrobial silver is coordinated by bioligands, as it has a very special, linear coordination preference in many cases. Furthermore, it is quite easily reduced to Ag°. We study how silver ions bind to peptides and proteins, under which circumstances silver ions are reduced and how the mechanisms of these processes influence living organisms. One of the studied organisms is Geobacter sulfurreducens, a bacterial strain that is used in water remediation and in bio-fuel cells. We also investigate how compounds with silver and other metal ions can be used to combat cancer and infectious diseases.

coordination compounds and polymers with interesting physical and biological properties, ranging from white light emission via sensing to controlled release

In terms of infrastructure and analytics, we frequently use single crystal structure ICP-OES S as well as the cellular and bacterial labs in the chemistry department.

Our group is an international, multi-cultural and diverse bunch of great young people with many different expertise.



## Fromm

### Group



New Antimicrobial Strategies Based on Metal Complexes, Mickaël Claudel, Justine V. Schwarte and Katharina M. Fromm,

Chances and challenges of long-distance electron transfer for cellular redox reactions Bernd Giese, Maksym Karamash and Katharina M. Fromm.

Stimuli-Responsive and Antibacterial Cellulose-Chitosan Hydrogels Containing Polydiacetylene Nanosheets Edwin S. Madivoli, J. V. Schwarte, Patrick G. Kareru, Anthony N. Gachanja, Katharina M. Fromm, Polymers 2023, 15(5), 1062

WEBSITE: http://frommgroup.ch/



CRYSTALS

**E**FFLUX PUMP

FERROCENE

GEOBACTER SULFURREDUCENS

HOPPING OF ELECTRONS

NORGANIC

KATHARINA

LITHIUM ION BATTERIES

MESOPOROUS SIO



ANORATTLES OPTICAL PROPERTIES

PEPTIDES & PROTEINS -BAND

DILVER **T**UNABLE PROPERTIES

UNDERSTANDING

VERY EXCITING

WHITE LIGHT EMISSION

-RAY DIFFRACTION

STANDS FOR TYROSINE

OUTER MEMBRANE CYTOCHROME OmcZ



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### POLYMER CHEMISTRY

## New mechanisms for the synthesis of highly defined polymers

# Prof. Andreas

So long, and thanks

for all the fish

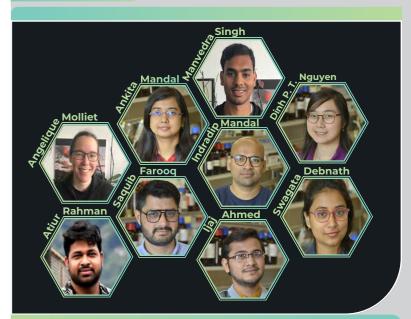
The Kilbinger Group is mainly involved in the preparation of polymers. Polymers are long, typically linear, molecules consisting mostly of one but sometimes also of several different repeating units. Polymers have become an indispensable part of our everyday life. They perform a multitude of very different tasks, whereby most polymers have a rather banal function, namely that of filling space with mass. However, some polymers also have very demanding tasks to perform, e.g. by protecting drugs from breaking down too quickly in the body or from undesired immune responses. Others can change their properties depending on external influences such as temperature or light. In such highly specialised polymers, it is often important to have a large degree of control over the length, the sequence of repeating units or the chemical structure of the chain ends during synthesis. KILBINGER This requires a very detailed understanding of the polymerisation mechanisms. Only with such knowledge can new polymerisation methods be found or even better defined polymers be produced.

> The Kilbinger group is working on the development of such polymerisation mechanisms in relation to two very different groups of polymers. On the one hand, we are developing new polymerisation methods in the field of ruthenium carbene complex catalysed olefin metathesis polymerisation. On the other hand, new processes are being investigated that make it possible to incorporate step-growth polymers such as Kevlar in a defined way into other polymers or to produce tube-like polymers with antimicrobial properties.



# Kilbinger

### Group

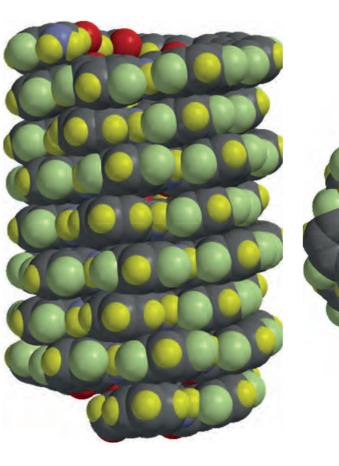


Catalytic Living Ring-Opening Metathesis Polymerization using Vinyl Ethers as Effective Chain Transfer Agents Mandal, A.; Mandal, I.; Kilbinger, A.F.M. Angew. Chem.. 2023, 62, e202211842

A Practical Route for Catalytic Ring **Opening Metathesis Polymerization** Mandal, I.; Kilbinger, A.F.M.

Chain Transfer Agents for the Catalytic Ring Opening Metathesis Polymerization of Norbornenes Mandal, I.; Mandal, A.; Rahman, Md A.; Kilbinger A.F.M.

WEBSITE: https://homeweb.unifr.ch/kilbinge/pub/



Model of a tube-like polymer as described above

### COLLOIDAL PHYSICAL CHEMISTRY

## **Controlling the shape of polymer colloids**

## Prof. Marco LATTUADA

### Let's get colloidal particles into (non-spherical) shape!

Polymer colloids are among the most well-studied, abundantly researched, and best-understood systems in colloidal science. Their application range includes paints, coatings, production of bulk polymer commodities, drug delivery vehicles, and packing materials in chromatographic columns, to mention some of the most important commercial uses. Polymer colloids have also significantly contributed to the understanding of the fundamentals of colloidal science, as they have been used as large-size equivalents of atoms and have helped physicists expand the theory of phase transitions. They also contributed to reaching a better understanding of phenomena such as crystallization and glass transition and have, therefore, significantly contributed to the development of soft matter science.

progressively better control of the composition, size, and internal structure of polymer colloids. However, there is one additional crucial parameter that is much more difficult to control: the shape of colloids. Despite the enormous benefits that emulsion and precipitation-based techniques offer, they almost inevitably lead to spherical particles because the sphere is the one shape that minimizes the surface, and consequently the interfacial energy, of a particle with a given volume.

Our group has recently made some exciting developments in this respect. We have developed a robust method to control the shape and functionality of polymer colloids. We have extended an old particle synthesis protocol, the activated swelling method, commercially used to prepare core-shell functional particles and modified it to prepare a wide variety of functional particles with two faces (Janus particles), having different compositions: polystyrene and polymethacrylates. Various particles have been prepared, ranging from spherical Janus particles to dimpled and half-spherical particles. Further manipulation of these asymmetric particles using solvents that can selectively dissolve one of the polymers leads to the formation of disk-like particles, mushroom-shaped particles, and colloids with one or two dimples. Further extensions of the method have led to dumbbells and particles with two small patches. SEM images of some of these particles are showcased in the figure. These functional particles have exciting properties: colloidal surfactants, colloidal molecules, and self-propelled microbots. The sphere was the perfect shape according to the ancient Greeks, but it was time to move beyond it!



## Lattuada

### Group



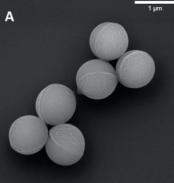
Controlling the morphology of polystyrene dumbbell particles Kata Dorbic and Marco Lattuada, Colloids and Surfaces A,

Preparation of Non-spherical Janus Particles via an Orthogonal Dissolution Approach Giovanni Russo and Marco Lattuada, Macromolecular Rapid

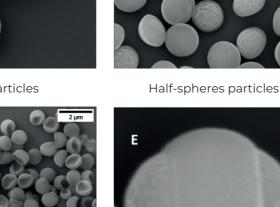
Synthesis of dimpled polymer particles and polymer particles with protrusions–Past, present, and future Kata Dorbic and Marco Lattuada, Advances in Colloid and Interface

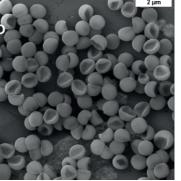
WEBSITE: https://www.unifr.ch/chem/en/research/groups/lattuada/

SEM images of various non-spherical polymer colloids.



Janus particles

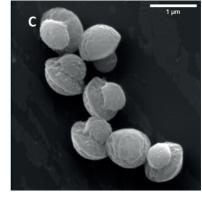




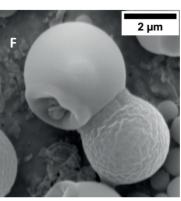
**Dimpled** particles



Two-patches particle



Mushroom particles



Dumbbell particles

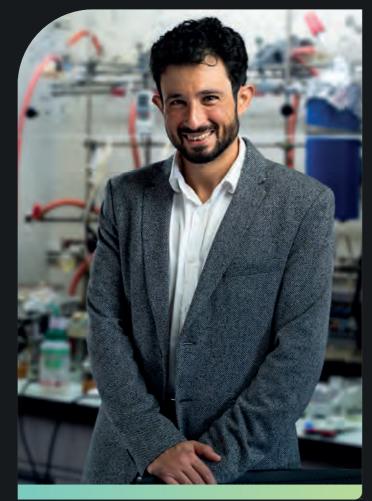
### ARTIFICIAL PHOTOSYNTHESIS

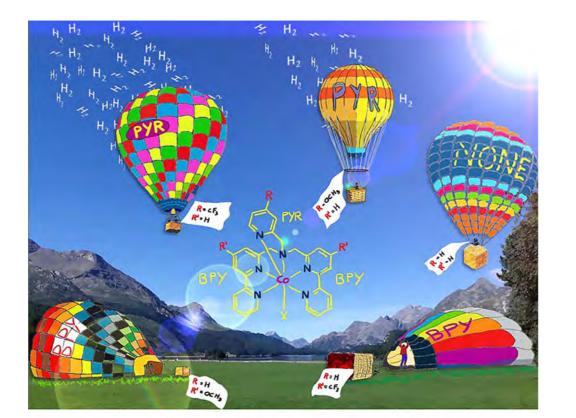
## Making solar fuels: water splitting and beyond

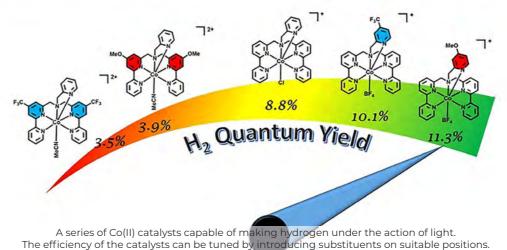
Dr. Albert RUGGI

Shine on you crazy ...catalyst The quest for alternative sources of energy is emerging as a crucial component of our journey towards a sustainable and carbon-neutral future. Solar fuels (like molecular hydrogen or organic molecules derived from the reduction of CO<sub>2</sub>) are a class of compounds capable of storing and releasing the energy contained in sun light. These innovative energy carriers have the potential to reshape our energy landscape, offering a clean and renewable source of power while mitigating the environmental consequences of traditional fuels. The conversion of sunlight into solar fuels is a process called artificial photosynthesis, because it is analogous to the natural process of converting water and CO<sub>2</sub> into sugars and other energetic molecules. Catalysts are essential for solar fuels production because they enhance energy conversion efficiency, improve reaction kinetics, control product selectivity, enhance system stability, and make solar energy storage and utilization more practical and sustainable. Their development and optimization are critical for advancing the field of solar fuels and promoting the transition to a more sustainable energy future.

Our group works on the development of catalysts to photochemically produce hydrogen and organic compounds derived from the reduction of  $CO_2$ . To make our systems sustainable, we use earth-abundant metals, like cobalt and iron. We are not only synthesizing these catalysts but also investigating in detail their catalytic mechanism together with our network of national and international collaborators. In this way, we learn how to design new species with optimized performances. We have recently developed a series of cobalt catalysts with an exotic structure, which is associated with remarkably high activity towards photochemical hydrogen production. Very recently, we have observed that replacing cobalt with iron we can obtain catalysts capable of reducing  $CO_2$  with a very high efficiency and selectivity. In both cases, investigation of the mechanism suggests that the localization of the electrons upon catalyst reduction plays a crucial role. We are now developing new catalyst including tailored redox-active ligands. Stay tuned!

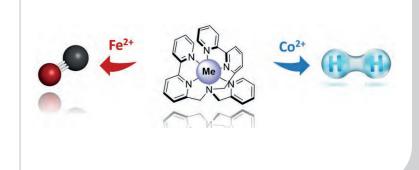






Ruggi

Group



#### Recent publications:

### Electro-and photochemical $H_2$ generation by Co(II) polypyridyl-based catalysts bearing ortho-substituted pyridines

F. Lucarini, J. Fize, A. Morozan, F. Droghetti, E. Solari, R. Scopelliti, M. Marazzi, M. Natali, M. Pastore, V. Artero, A. Ruggi, Sustainable Energy and Fuels 2023, 7, 3384-3394.

### Rethinking Electronic Effects in Photochemical Hydrogen Evolution Using CuInS<sub>2</sub>@ZnS Quantum Dots Sensitizers

A. Orlando, F. Lucarini, E. Benazzi, F. Droghetti, A. Ruggi, M. Natali, Molecules 2022, 27(23), 8277.

#### Rationalizing Photo-triggered hydrogen evolution using polypyridine cobalt complexes: substituent effects on hexadentate chelating ligands

F. Lucarini, D. Bongni, P. Schiel, G. Bevini, E. Benazzi, E. Solari, F. Fadaei-Tirani, R. Scopelliti, M. Marazzi, M. Natali, M. Pastore, A. Ruggi, ChemSusChem, 2021, 14, 1874-1885.

WEBSITE: https://www.unifr.ch/chem/en/research/groups/ruggi/

### BIOCOLLOIDS

## **Physical Chemistry for Food and Health**

Our research group is dedicated to exploring the fundamental principles of colloid and interface chemistry. We examine colloidal structures as functional units in nature's materials, finely tuned by millions of years of evolution. We apply these concepts to create new materials that foster molecular, structural, and cellular interactions. Our vision is to pioneer innovative, multi-functional materials with far-reaching impacts across diverse domains, including food science and MedTech.

### Research

## Prof. Stefan SALENTINIG

Our recipe for success: Passion for science, curiosity, creativity, and caffeine! Our research activities encompass a wide spectrum, ranging from directed self-assembly and disassembly processes that facilitate the creation of cutting-edge supramolecular materials in food and health science. We employ in-situ and in-operando techniques in our laboratory and at synchrotron facilities. Our state-of-the-art experimental methods are at the core of our material design and characterization efforts. We have established a unique meso- and nanoscale characterization platform in Switzerland. We operate a MetalJet small-angle X-ray scattering system, spectroscopic imaging ellipsometry, confocal Raman microscopy, and multi-angle light scattering. When existing techniques fail to address our research questions, we develop custom methodologies tailored to our needs.

#### Training of Students and Young Scientists

In parallel to our research, we are committed to teaching and training the next generation of scientists in an interdisciplinary environment exposed to highly contemporary experimental methods. Over the last two years, several students have received training and worked at synchrotron and neutron sources in Switzerland, Italy, France, and the UK. We also have strong international connections for PhD and postdoc exchanges with various institutions. Examples include PhD student exchanges with the University of Sao Paulo in Brazil, the University of Umea, Sweden, NTU in Singapore. Additionally, we have hosted summer internship students from our university, the University College London, the University of Chicago, the University of California Berkeley, and more.

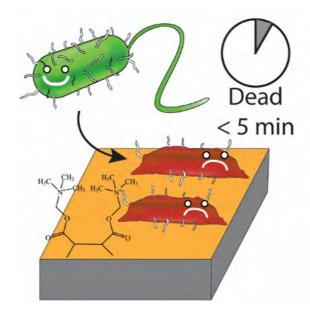
#### Alumni 2022-2023 with Career Progression

Several students have graduated and advanced in their careers over the past two years. Dr. Linda Hong is now a lecturer at NUS in Singapore, Dr. Samuel Watts has moved to NTU in Singapore as a postdoc, Dr. Mark Gontsarik became postdoc at the University of Ghent in Belgium, Dr. Mahsa Zabara is Vice President for Research at Livinguard AG in Zug, Switzerland, Dr. Andrea Lassenberger is Application Lab Head at Xenocs AG in France, and Dr. Marco Manca started as a process engineer at Evatec AG in St. Gallen.

### Outreach

We have several partnerships with the food and antimicrobial/pharma industry, organized workshops and seminars (e.g., the SAXS workshop featured separately in this report), contributed to several conferences, and received multiple best presentation and poster awards. We co-edited a special issue on Food Hydrocolloids in Current Opinion in Colloid and Interface Science in 2023. Our contributions extend beyond the laboratory as we actively engage with the wider community by participating in media panels, newspaper articles, and radio interviews.





We developed functional, self-disinfecting surfaces and antimicrobial nanomaterials for various applications in the food and health sectors.



We created novel food emulsions from whey proteins and buriti plant oil, naturally rich in unsaturated fatty acids, vitamins, and antioxidants.

# Salentinig

## Group



### **Recent publications:**

Structure Formation in Tailor-Made Buriti Oil Emulsion During Simulated Digestion Freire, R. V. M., Hong, L., Peterek, M., Canarelli, S., Rezzi, S., Salentinig, S., Adv. Funct. Mater. 2023, 2303854. https://doi.org/10.1002/adfm.202303854

Supramolecular design of CO2-responsive lipid nanomaterials, Journal of Colloid and Interface Science Debas M., Freire R. V. M., Salentinig S., 637, 2023, 513-521, https://doi.org/10.1016/j.jcis.2023.01.060

Human Antimicrobial Peptide Triggered Colloidal Transformations in Bacteria Membrane Lipopolysaccharides Hong, L., Gontsarik, M., Amenitsch, H., Salentinig, S., Small 2022, 18, 2104211. https://doi.org/10.1002/smll.202104211

WEBSITE: https://www.unifr.ch/chem/en/research/groups/salentinig/

### QUANTUM THEORETICAL LAB

# From rigorous theory to practical and robust quantum-chemical approximations

## Prof. Stefan VUČKOVIĆ

HΨ = EΨ as foundation, Al for acceleration, challenging chemistry for application Quantum-chemical simulations have become a powerful part of chemistry and material science research. In addition to enabling rationalization of experiments, these simulations have enabled major technological advances by predicting new drugs, reactions, catalysts, and functional materials. By reducing resources (time, money, energy) needed for experimental trial-and-error procedures, quantum simulations have the potential to enable dramatic speed-ups in chemical discovery and technological advancements. Our group focuses on the key quantum chemistry challenges:

### 1. Solving the Strong Correlation Problem in Density Functional Theory

Work in this area focuses on developing fundamentally novel models for strong correlation within density functional theory (DFT). Strong correlation happens when electron interactions in molecules are too complex for standard DFT models to accurately predict their behavior. Our goal is to solve long-standing problems and unlock the full potential of DFT for discovery of transition metal catalysts and functional materials. We approach the strong correlation problem by using the exact foundational theory to expand the mathematical space for building DFT approximations. Then we explore this new space with the help of artificial intelligence (AI) models to create robust approximations for accurate chemical predictions.

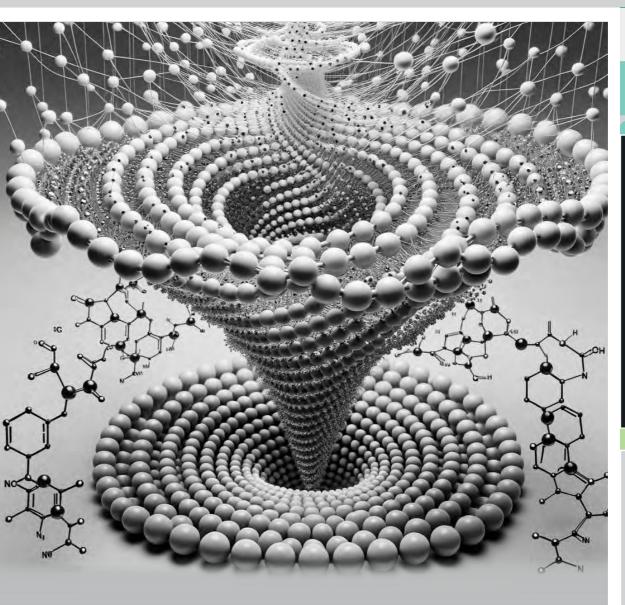
### 2. Accurate simulations of noncovalent interactions

Noncovalent interactions play a crucial role in a variety of fields including biology, chemistry, material science. We aim to transform simulations of noncovalent interactions by using pure electronic structure models, intended to replace the heuristic methods presently employed in quantum chemistry for these interactions. Our efforts already enable highly accurate simulations of large complexes, electron transfers, and unseen complexes. These efforts complement our work on strong correlations, as we aim to expand quantum chemistry's capabilities by creating a robust framework that consistently addresses both strong electron and noncovalent interactions.

### 3. Divide and conquer quantum-chemical errors

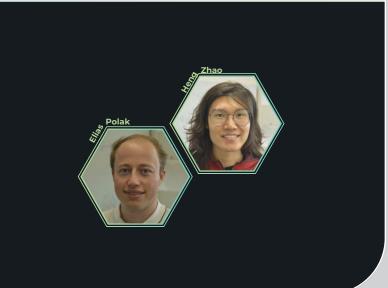
Quantum-chemical simulations contain multiple sources of errors due to the sets of approximations involved. The group develops tools, indicators, and accuracy predictors to identify and analyze these error sources independently, leading to a better understanding and reduction of errors and greater accuracy of simulations in chemistry and surface science.





## Vučković

### Group



#### Selected publications:

Regularized and Opposite Spin-Scaled Functionals from Møller–Plesset Adiabatic Connection–Higher Accuracy at Lower Cost. The Journal of Physical Chemistry Letters

Daas, K. J.; Kooi, D. P.; Peters, N. C.; Fabiano, E.; Della Sala, F.; Gori-Giorgi, P.; Vuckovic, S. 2023, 14, 8448–8459.

Nonlocal Functionals Inspired by the Strongly Interacting Limit of DFT: Exact Constraints and Implementation. Journal of Chemical Theory and Computation Vuckovic, S: Bahmann, H. 2023, 19, 6172–6184.

**Extending Density Functional Theory with near Chemical Accuracy beyond Pure Water. Nature Communications** Song, S.; Vuckovic, S.; Kim, Y.; Yu, H.; Sim, E.; Burke, K. 2023, 14.

VEBSITE: https://www.stefanvuckovic.com

### INORGANIC MEDICINAL CHEMISTRY

## **Rare metal chemistry to the discovery** of new pharmaceutical agents

Prof. Fabio ZOBI

In metallis raris solutiones unicae ad medicinam

Medicinal chemistry is discipline at the intersection of chemistry and pharmacology and other biological specialties, aiming at the design, chemical synthesis and development of pharmaceutical agents, or bio-active molecules. Inorganic chemistry is the science dedicated to the preparation of metalbased substances in the laboratory. Thus, inorganic medicinal chemistry is a discipline dedicated to the preparation and study of metal-based molecules of pharmacological interest. Our group's interest and aim is to develop new chemistry of rare metal ions and consequently discover new molecules and reactivity of the same for medicinal applications. We focus in particular on the preparation of anticancer and antimicrobial agents and carbon monoxide releasing molecules as both cytotoxic and cytoprotective molecules. We devote particular attention to colorectal carcinoma (CRC) and methicillin-resistant Staphylococcus aureus and Candida infections. In parallel to these studies, we are also interested in the design and preparation of natural bio-carriers as delivery agents of our metal-based drugs. In particular, we use environmentally friendly, abundant and safe microalgae in their diatom form as delivery capsules for inorganic and organometallic antitumor agents. Tumour specificity of these materials is realised via functionalization of their surface with vitamin B12.

cancer deaths in 2018) and the concurrent emerging threats of antimicrobial resistance and invasive fungal infection, our line of research falls within the WHO recommendations of new solutions outside the traditional development pathway, with emphasis on new active compounds with non-classical mechanisms of action. To be able to reach our long-term goals of finding viable solutions for the above-mentioned pathologies, we approach the problem from both an academic and practical side: a) academically we develop new reactions to access unusual structures and properties of the metal complexes. b) from a more practical side, our group has established a long-term collaboration with the Institute of Molecular Genetics and Genetic Engineering of the University of Belgrade where the new substances we prepare are tested in vivo on clinical isolates derived from patients currently under hospital care.



# Molecular Library Re Pt **Active Compounds** S. aureus MRSA 43300 10 8 6 4

C. albicans nfection in vive Properties Drug-Likeness MRSA = 0.8 µM (635 ng/mL) ReNN3P C. albicans = 6.2 µM (1 × MIC) Therapeutic index > 47 Effective both in vitro and in vivo t and Metastasis in HCT.116 Tum 1 2 5 114 (1/2) LARGE THERAPEUTIC INDEX TRIPLE ACTIVITY IN VIVO

Zobi

### Group

< 1.5 µM

3.1 μM 6.2 µM 12.5 µM

> 12.5 µM

< 1.5 µM

3.1 µM

6.2 μM

12.5 µM

> 12.5 µM

IC50, MIC

**Toxicity Profile** 



Combatting AMR: A molecular approach to the discovery of potent and non-toxic rhenium complexes active against C. albicans-MRSA co-infection. I.S. Nasiri Sovari, N. Radakovic, P. Roch, A. Crochet, A. Pavic, F. Zobi; Eur. J. Med. Chem., 2021, 226,113858.

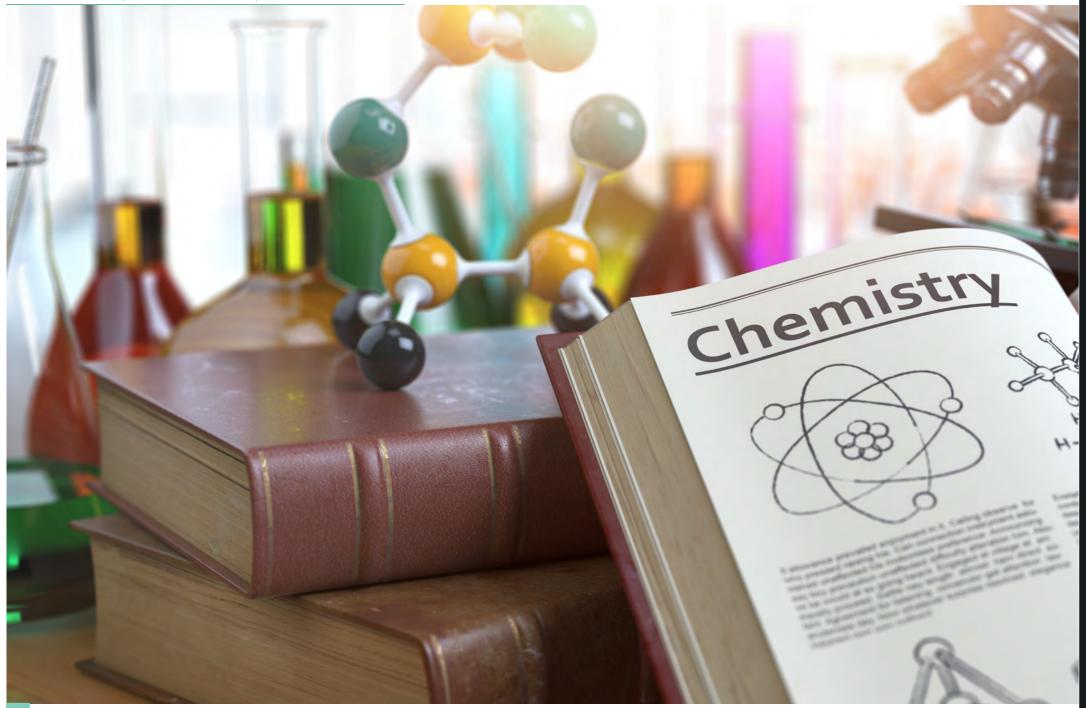
Identification of novel potent and non-toxic anticancer, anti-angiogenic and antimetastatic rhenium complexes against colorectal carcinoma. J. Delasoie, A. Pavic, N. Voutier, S. Vojnovic, A. Crochet, J. Nikodinovic-Runic, F. Zobi; Eur. J. Med. Chem., 2020, 204,112583.

Design, synthesis and in vivo evaluation of 3-arylcoumarin derivatives of rhenium(I) tricarbonyl complexes as potent antibacterial agents against methicillin-resistant Staphylococcus aureus (MRSA).

S. Nasiri Sovari, S. Vojnovic, S. S. Bogojevic, A. Crochet, A. Pavic, J. Nikodinovic-Runic, F. Zobi, Eur. J. Med. Chem., 2020, 205,112533.

WEBSITE: https://fabiozobi.wixsite.com/zobigroup







UNIVERSITY OF FRIBOURG | DEPARTMENT OF CHEMISTRY | 2021-2022



**Bachelor student** 

J'ai choisi d'étudié la chimie car c'est une science qui nous perme d'expliquer le fonctionnement du monde qui nous entoure. De plus, la chimie a un impact significatif sur notre vie quotidienne en agissant sur plusieurs secteurs diffèrent comme la médecine, la science des matériaux, l'industrie agroalimentaire et aussi d'un autre côté de résoudre des problèmes environnementaux. J'a toujours été fasciné par la diversité des domaines d'applications de cette branche.

De mon point de vue, étudié la chimie à l'université de Fribourg est très enrichissante car on a la possibilité de suivre un cursus bilingue. En outre, la proximité avec le corps professoral et la cohésion entre les étudiants offre un environnement de travail motivant et conviviale. En effet, l'association des étudiants de chimie contribue à la bonne convivial au sein de l'université ainsi que de la vie estudiantine à Fribourg.

Le cursus de l'université de Fribourg offre un large panel de compétences à la fois pratiques et académique complet via des travaux pratique ainsi que des cours permettant d'avoir les outils nécessaires afin d'enrichir son bagage de connaissances.

La variété des sujets étudier dans les différents groupes de recherches offre la possibilité de découvrir divers domaines de la chimie dans lesquels se spécialiser à la suite du cursus académique.



Baptiste Chapuis Master student

Since I was little, I have always been fascinated by documentaries describing natural phenomena. In high school I truly developed an interest in life sciences and, while all of them interested me, hemistry came rather naturally, and that is why I decided to pursue a Bachelor's degree in chemistry.

Studying chemistry at the University of Fribourg was for me an ndoubtable choice. Although it is close to where I live, this was not the main argument that justified my choice. In fact, I did a lot of research beforehand to establish which of the many Swiss niversities was the best fit for me and for what I believe in.

The Department of Chemistry at the University of Fribourg is not nown as one of the biggest. In my opinion, this is exactly what makes the teaching experience so great and so unique. Since there are only a few students per year, we manage to build a strong network with fellow colleagues.

Furthermore, it is truly a privilege to have close relationships with the Professors, who are valuable and renowned assets to the faculty. Because we are a small unit, as students, we can turn to them for any question or doubt, and they are always open for a chat in the hallwavs

Overall, I am very satisfied with the background knowledge I received during my Bachelor's, but it was not enough for me. That is why I decided to embark on a Master's degree here in Fribourg. During our studies, we have to follow compulsory lectures, for which I am quite grateful. Although they might be outside of one's interests, they could attest to a broad skill range, solid foundations for a future job and, why not, lead us to a new passion.



NGUYEN Dinh Phuong Trinh PhD student

In our daily lives, in nature, everywhere, chemistry does its job, and what a job! It is the basis of vital processes, and its understanding has enabled us to make many technological advances in combination with other applied sciences. There are numerous areas to explore in chemistry, such as analytical chemistry, physical chemistry, materials chemistry, and my personal favorite, organic chemistry. The latter is used to study the structure and transformation of organic molecules found in cosmetics, food, and plastics for instance.

At Fribourg, I was able to start my PhD in a subject that combines organic and polymer chemistry. In my day-to-day life, I plan reactions, run them, purify products I obtain then analyze them. We can draw inspiration from Nature to create artificial products in our laboratories that may be useful later. In this case, the polymers I synthesize form helices that mimic the natural helices found in DNA, RNA, and proteins to cite a few examples. There are still a lot of mysteries to unearth in this field, but that is what makes this journey exciting!

Despite the small size of the University of Fribourg, the quantity and quality of the equipment available on-site is impressive. This means one can carry out highly advanced research in a friendly atmosphere, whether with students, other researchers, or professors. With its vastly diverse research fields, the chemistry department sits in close proximity to the departments of biochemistry, medicine, and physics, which is an advantage for idea sharing and collaboration. The doctoral journey is incredibly enriching, as it provides both a development of personal and professional skills as well as a deep understanding of the matter you work on

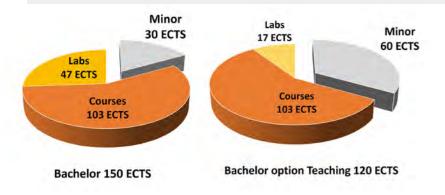
# **Virtual Reality Approach** for Chemistry Education

Aurélien

The chemistry department has recently integrated a Virtual Reality approach to improve the accessibility and understanding of chemical concepts and structures. In this perspective, 20 HTV Vive Focus 3 headsets were acquired and used to access the Nanome software, which provides a unique interactive interface where the students can draw structures, modify them and visualize them in 3D. Members of the chemistry department have shown strong commitment to adopt of virtual reality. Overall, the integration of the VR experience into our teaching environment is expected not only to provide a strong benefit for the students, but also further strengthen the standing of our University as an innovative institution that makes use of state-of-the-art teaching methods and tools.

# Study Program

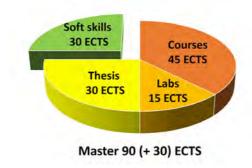
Everything around us, including ourselves, is made up of atoms and molecules. The ability to create new materials and compounds, to analyse their behaviour and to modify them according to our needs, is the basis of research in chemistry. However, to meet the challenges of the future, it is necessary to have a sound background: for this reason, the Department of Chemistry has a strong focus on teaching at all levels, from Bachelor to Master to Doctorate. thanks to an extremely favourable student/teacher ratio, we can take care of our students at an individualised level.



At the Bachelor level, we offer a Major program (Branche Principale, Hauptfach) of 150 ECTS over 6 semesters, complemented by a Minor (Branche complémentaire, Zusatzfach) of 30 ECTS of the student's choice. For students interested in teaching in the Secondary School, we also propose a 120 ECTS Major program (Chimie: option enseignement, Chemie: Option Lehren) to be complemented by a Minor of 60 ECTS of the student's choice This division enables students to explore different fields and to keep a high level of flexibility. Just to mention some examples, popular Minors are Industrial Chemistry (proposed by the HES-SO Fribourg) and Minors offered by the Faculty of Science (Biology, Biochemistry, Physics, ...). Minors offered by other Faculties within the University of Fribourg are also possible. The Major in chemistry of 90 ECTS nicely complements theoretical and practical courses: didactic laboratories constitute more than 50% of the total ECTS. The students will gain first hand practical experience in all fields of chemistry, including Analytical Chemistry, Organic Synthesis, Physical chemistry,... A project (Bachelor Projects) conducted in one of the research groups will also provide the students with a first experience of scientific research. The Major in Chemistry for Teaching of 60 ECTS is more focused on the theoretical courses, with circa 30% of didactic laboratories.

Bilingualism constitutes a strong asset of our teaching: Bachelor classes are taught in French or German (according to the choice of the teacher), whilst the exams can be done in French or German, according to the student's choice. The written exams of the first year and some exams of the second and third year can be done also in Italian. Bilingualism is mentioned on our B.Sc. diplomas.

At a Master level, we offer a 90 ECTS program over 3 semesters. The study plan is divided between a core block of compulsory courses (42 ECTS) complemented by a series if elective courses (18 ECTS). This combination allows students to follow their own inclinations and interests, providing at the same time a strong common background on advanced topics. To make students capable of with advanced research topics. courses and exams take place in English.





The Master is also strongly focused on the practical courses: a module of 15 ECTS consisting of an advanced multidisciplinary didactic laboratory and two research projects (100 hours each) will enable students to get familiar

interacting in international environments, the The Master thesis (30 ECTS) is the culmination of undergraduate studies: the students will spend an entire semester in a research laboratory of their choice, interacting with the researchers, applying their theoretical knowledge to real-life cases, and strengthening their practical skills. An extra Soft Skill module (30 ECTS) has been recently introduced, providing in-depth formation on transversal competencies, including scientific writing, entrepreneurship and experimental design.

> The Department of chemistry is actively involved in the training and formation of Doctoral (Ph.D.) students, both in their research activity and in their theoretical formation. Seminars, summer schools and lectures given by invited speakers are regularly organized during the year.

# **The Leonardo** Program

### Following the path of the Mathematics department, Chemistry department also set up an honour program for outstanding high school students.

The Leonardo program, called after Da Vinci, allows talented students to follow University courses during their regular high school years. At the end of each semester, they are allowed to register to the course exam, and if they are successful, the corresponding ECTS credits are obtained and can be kept if they decide to enrol later at the University of Fribourg. In the (unfortunate and we hope unlikely) case the exam is not successful, the attempt is not registered, and has no impact on their later studies at the University.

It is of course a significant additional effort for the students, and it may have consequences on other topics in the high school curriculum. For that reason, the progress of the student on both the University and the high school is closely monitored, and if warning signs are identified, a discussion with the student and both institutions will take place to figure out the nature of the problem. If, for any reason, the student drops out of the program, she/he is anyway allowed to try it again the following year. Similarly, the student is allowed to follow the classes and not register for the exam.

Three students joined the program since its initiation in the Fall of 2022. One of them decided to drop out quite early; one of them succeeded very well and is now a regular student, and one of them is currently following it.

proposés ont apporté des compléments, des détails parfois les concepts étudiés et les applications concrètes, dans la nature comme dans l'industrie, sont mis en évidence. la curiosité et l'engouement pour la chimie.

La mise en place d'une redoutable organisation a été un réviser et rattraper les cours manqués. Il est toutefois un apprentissage extrêmement utile pour la suite des études universitaires comme gymnasiales. Organisation, dit gain de temps, dit responsabilisation et efficacité plus grande. L'entrée à l'université se fait avec une assurance plus grande, car nous avons acquis une méthode de travail à notre image et une capacité de travail en autodidacte.

à l'université, cette immersion est la chance unique de mesurer la différence entre le secondaire II et l'université Le choc face à des cours plus compacts, lourds et rapides de l'université force à l'adaptation et diminue l'incertitude lors de la transition d'un univers à l'autre. Le programme à l'université et d'être assuré qu'il s'agit réellement de ce vers quoi nous désirons nous diriger. Ainsi, ce programme aptitude à étudier efficacement.

L'engouement pour la chimie et les cours ont contribué Le programme Léonardo a été une préparation à la complexité de certains problèmes et sujets peu couverts par le gymnase ce qui facilite une qualification. Pour ma part (Laura), le programme a réellement été un tremplin vers une passion, une curiosité que je me suis



compétition. Les week-ends de préparation proposés par l'association ont été un approfondissement supplémentaire dans la natière et surtout la rencontrer avec les projets concrets de PhD, es étudiants, des chercheurs, d'autres gymnasiens. Ce parcours à Zürich ce qui ne m'a pas empêché de m'engager durant le Olympiades internationales. J'y ai travaillé en laboratoire en tan Le programme Léonardo m'a permis de découvrir une curiosité pour la chimie et m'a motivée à saisir les opportunités d'en apprendre plus tout en me donnant les clés pour réussir dans les

que le progamme Léonardo a à offrir en matière d'apprentissage. '

Laura Ratano (left). Collège du Sud Jinhyao Han (right), Collège Sainte-Croix



KidsUni, Swiss Young Researcher, WINS (Women In Science And Technology) and other collaborations with various schools.



The Chemistry Department of the University of Fribourg offers large groups of visitors the opportunity to attend entertaining shows on the subject of CHEMISTRY. We use the ideas as an interactive tool to give children, as well as adults, a first impression of science and chemical experiments. Every Christmas, Prof. Katharina Fromm, with the support of many different members of the institute, is launching a new spectacle full of chemical experiments, smoke and color! She had set up so many different performances up to today.

## **Public Outreach**

The MINT program (Mathematics, Computer Science, Science and Technology) has set itself the goal of providing all pupils; including children from the primary school age, but also high school students, a first access to science regardless of their professional future. The program is being implemented by the members of the Chemistry Department of the University of Fribourg and the Adolphe Merkle Institute. It is co-financed by the Swiss Academy of Arts and Sciences.

### **Branches of MINT:**

### **Chaim Weizmann Lectureships:**

Chaim Weizmann Lectureship is founded at end of 2009 with the idea to promote chemistry and the standpoint of the Department of Chemistry in Fribourg. It consists of inviting a well-known personality from the area of Chemistry for a lecture to Fribourg for ca. 2-5 days. The guest speaker has the opportunity to discuss with members of the University community and to visit Fribourg and its region. Department of Chemistry hosted so many well-known professors.

### **Chemistry Shows:**

### Explora / Open Doors Day:

University of Fribourg offered the third edition of its Open Doors and Explora events to the general public and to the members of the community in the fall 2023. A day of sport, meetings, science and culture that brought together nearly 2,500 visitors on the Plateau de Pérolles.







SAXS

### **First Metaljet SAXS Installation in Switzerland** in the Department of Chemistry

A SAXSPoint 5.0 with MetalJet X-ray source from Anton Paar, the first of its financed with an integrated approach involving the NCCR Bio-inspired Materials, Frimat, the Faculty of Science and Medicine, the Department of Chemistry, and group funding. The equipment allows state-of-the-art X-ray scattering and diffraction experiments on liquids, solids, and surfaces. It offers high temporal and spatial resolution previously inaccessible in the laboratory setting. The set-up is key for the ultrastructural analysis of materials, a key aspect of, for instance, (bio)material chemistry, polymer chemistry, nanomaterials, and food- and pharmaceutical sciences.

The capabilities of the set-up include (i) ultra-low-angle SAXS and WAXS to study structural properties from the angstrom range up to around 500 nm; (ii) grazing incidence SAXS and WAXS to characterize structures in surfaces and interfaces under environmental conditions and solvent; (iii) high temporal resolution for in situ and operando studies with minute resolution required to study stimuli-induced structural rearrangements in nanomaterials. It significantly contributed to PhD and Postdoc training in characterization capabilities in Fribourg, and became a crucial asset for multiple projects across and beyond the Department.



### Inauguration Workshop at the Department of Chemistry

To celebrate the inauguration of the first metallet SAXS system in Switzerland, we organized a workshop entitled "A Journey to the Heart of Matter" at the Department of Chemistry, University of Fribourg, on April 21, 2023.

The workshop brought together leading material scientists from academia and industry. The conference aimed to foster a platform for exchanging ideas and knowledge on material science for health and food applications.

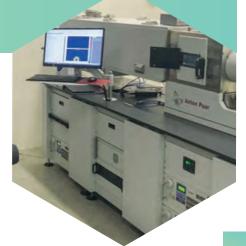
We had the pleasure to welcome the following speakers: Prof. Alex Dommann (Empa and University of Bern), Dr. Andreas Keilbach (Anton Paar), Prof. Paola Luciani (University of Bern), Dr. Martin Leser (University of Fribourg), Dr. Hans-Jörg Limbach (Nestlé Research).





The inauguration provided an excellent opportunity for researchers and students to network and engage in discussions on the potential of SAXS in material science and the future of the field. The conference and inauguration were highly successful events that brought together key material scientists from academia and industry to share their knowledge and insights on the SAXS technique and mark a historic moment that will undoubtedly lead to many discoveries and applications in materials chemistry.

A momentous occasion as our distinguished guests - the State Councilor Sylvie Bonvin-Sansonnens, the future Rector Prof. Katharina Fromm, and the Chair of the event (from left to right) - join us to celebrate the inauguration of our new MetalJet SAXS, with a chocolate model for the apero. Right: Demonstration of the MetalJet SAXS in the laboratory with Nataly Viens Python, Director of the Haute Ecole de Santé (from behind), Laurent Dietrich, Vice-Syndic of the City of Fribourg, Serge Rezzi, CEO of the Swiss Nutrition and Health Foundation, and State Councillor Sylvie Bonvin-Sansonnens.



## **X-Ray Service**

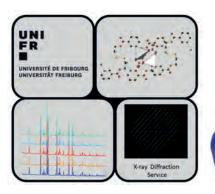
The X-ray diffraction service of the Chemistry department of the University of Fribourg, built up by Prof. K. M. Fromm since 2006, is equipped with different single-crystal diffractometers (Mo, Cu and Ag radiation) and two powder diffractometers (Cu-K αl and Cu-Kα radiation). Dr. Aurélien Crochet is in charge of the service, provides single crystal structure determination service and assistance and formation for the use of the powder diffractometer.

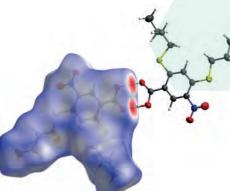
The application field is very large from organic molecules to inorganic and organometallic compounds. The single crystal service carries out measurement and full crystal structure determination. Apart from internal collaborations, the Crystallography lab offers its services also to research groups and industries at national and international level. Ready to publish CIF-files are provided and deposition to the CCDC is done on demand.

People who want to have access to one of the instruments have to contact the Dr. Aurélien Crochet in order to discuss about their needs.



More info and detail on machines on our website: https://www.unifr.ch/chem/en/services/platforms/x-ray.html





### **Recent publications and highlights:**

 Dalton Trans, 2023, DOI: 10.1039/D2DT04041G; J. Mol. Struc. 2023, DOI: 10.1016/j.molstruc.2023.136398.

 Acta Cryst. C, 2023, DOI: 10.1107/S2053229623005867; Inorganics, 2023, DOI: 10.3390/inorganics11040139,

 Antibiotics, 2023, 10.3390/antibiotics12030619; Acta Cryst. E, 2023, DOI: 10.1107/S2056989022003589;

 Nat. Prod. Res., 2022, DOI: 10.1080/14786419.2022.2056891; Molbank, 2022, DOI: 10.3390/M1504;

 Pharmaceuticals, 2022, DOI: 10.3390/ph15091107; J. Coord. Chem., 2022,

## MALDI

### (Bruker UltrafleXtreme MALDI-TOF)

This instrument is capable of measuring molecules of high molecular weight (1000-500000 m/z) and it is the standard instrument for polymer analysis. The access to this instrument is restricted. For details, please contact Dr. Albert Ruggi.



### NMR

## **HIGH FIELD NMR INSTRUMENTS**

## 600 MHz

The high-field 600 MHz Bruker Ascend magnet, under the precise control of the Avance NEO console, is enhanced with a liquid nitrogen-cooled dual broad-band (BBO) CRYO probe. This configuration enables exceptional sensitivity and delivers It is important to note this instrument is not available as open

## 500 MHz

Our 500 MHz Bruker magnet is managed by the Avance III HD console and is equiped with by SampeCase auto featuring 24 positions. Currently, the system is equipped v a 5mm BBO probe that includes Z-gradient. This probe is low as -150°C to as high as 150°C.

the NMR Service. However, upon special request, individuals



Our open access NMR instruments are accessible to proficient students. We have two systems available: a 400MHz Bruker Ascend and a 300 MHz Bruker Ultrashield, both managed using Avance Nanobay consoles. These instruments are equipped with high throughput 60-position autosamplers. Currently, they feature similar dual-channel 5 mm BBO probes with Z-gradient capabilities. These probes can be tuned over a frequency range suitable for observing nuclei ranging from <sup>31</sup>P and <sup>15</sup>N, as well as <sup>19</sup>F. Additionally, they allow for <sup>1</sup>H{<sup>19</sup>F} decoupled measurements.

500MHZ/52 MM

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## **OPEN ACCESS NMR INSTRUMENTS**

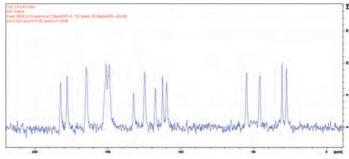
### **Open** access instruments 400 and 300 MHz

The 400 MHz instrument is further equipped with a BCU I temperature control unit, enabling NMR measurements at temperatures other than room temperature.

In essence, the instruments with their current probes are particularly sensitive for heteronuclear-detected methods, including APT, DEPT, and more. However, they also yield respectable spectra for 1H proton-detected NMR techniques such as 1D, DOSY, homonuclear 2D (COSY, NOESY, ROESY, TOCSY), and all inverse-detected methods (HSQC, HMBC, etc.).

Following an experiment, authenticated users can promptly download the collected spectra for subsequent processing and archiving.





### Solid-state MAS instruments 400 and 600 MHz

We currently operate two solid-state NMR instruments:

## 400 MHz

Our 400 MHz Bruker UltraShield magnet is controlled using the Avance Neo console and features a dual-channel BB probe. This setup allows for the acquisition of spectra from samples placed in 4 mm diameter rotors, enabling both single and double resonance experiments. If you're working with compounds that are insoluble or unstable in solution and require insights into their solid-state structure, this instrument is the ideal choice. It's capable of spinning samples at speeds ranging from 1 kHz to 15 kHz, and it supports the measurement of various nuclei, including <sup>1</sup>H, <sup>2</sup>H, <sup>6</sup>Li, <sup>7</sup>Li, <sup>13</sup>C, <sup>23</sup>Na, <sup>27</sup>Al, <sup>29</sup>Si, and <sup>31</sup>P via solid-state NMR.

## 600 MHz

The high-field 600 MHz Bruker Ascend magnet is controlled by the Avance NEO console and comes equipped with a "very fast" 1.3 mm MAS solid probe, capable of spinning samples at speeds of up to 67 kHz. This setup provides exceptionally high resolution for the analysis of solid samples.

## NMR FOR INDUSTRY

We extend an open invitation to external users to utilize our NMR systems for their sample measurements. After undergoing training, you have the option to independently prepare, measure, and analyze your own samples. Alternatively, if your time is at a premium, we can take care of these tasks on your behalf. Isn't that convenient?

### Try us out!

For further information and pricing, please get in touch with Dr. Krzysztof Piech.

## **Repair & Development**

With a long experience, the Electronics Workshop at the Department of Chemistry provides services to assist in the development, maintenance and safety of its research

It has a diverse range of equipment and facilities relevant to modern chemical science. Services provided are Consultancy & Advice / Design & Construction of Laboratory Equipment Maintenance & Repair, Machine Shop Facilities, stock of Electronic Components & Consumables. The skills in electronic and mechanical development are very high - from development to programming electronic cards and from drilling to machining parts. We are also proud that, over the years, we have accumulated experience in repair and maintenance of the majority apparatus used in chemistry.

For details, please contact Mr. Olivier Graber.

## **IT Support**

We provide any IT support that may be needed for science and research.

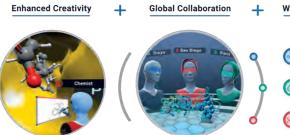
Our IT support developed extensive variety of services starting from basic IT support of our computers, data security, assistance during the installation of new equipment but also maintenance and service of our chemical equipment and development of diverse applications useful for our administration, machinery and data: Instrument Laboratory Management Access System, Integrated Database.

We are also very proud to be one of the first who have implemented VR classroom for our studies.

We train our personnel and students to move in virtual reality for science and research.

We are happy and open for new challenges in which we could combine our skills and new capabilities in big data analysis.

For details, please contact Mr. Wojciech Gajewski.







## **Synthesis Lab Service**

The Synthesis Laboratory was created in 2001, when the Institutes of Inorganic Chemistry, Organic Chemistry and Physical Chemistry merged to form the present

The synthesis laboratory was set up to support the department's professors and researchers, offering them help with the practical aspects of their research work. This support is provided by carrying out syntheses and all the preparations required to advance the projects of doctoral students and scientific collaborators in the various research groups. The laboratory is equipped with a wide rar and glassware, which are made available to researchers. The synthe also includes a hydrogenation laboratory, which currently enables r carried out at up to 50 bar.

Three employees supervise 6 apprentice chemists and have been providing practical training for many years. Through their daily supervision and support during analytical exercises, they have contributed to the training and success of 38 apprentices, who have obtained their Federal Certificate of Competence, more than 95% of them with an integrated vocational baccalaureate.

UNIVERSITY OF FRIBOURG | DEPARTMENT OF CHEMISTRY | 2022-2

## **IMPRESSUM & CONTACTS** CHEMISTRY DEPARTMENT UNIVERSITY OF FRIBOURG

## **DEPARTMENT OF CHEMISTR IGURES FOR 2022-2023** NATIONALITIES RESEARCHERS POSTDOCS PhD STUDENTS





**MSc STUDENTS** 

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**RESEARCH GROUPS** 

## COLLABORATORS







### **SNSF FUNDING**



### THIRD PARTY FUNDING







## Impressum

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## **Our contacts**

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