



SCS
Swiss Chemical
Society

SCS Fall Meeting 2024

September 5, 2024,

University of Fribourg, Campus Pérolles (PER 21 and PER 22)

Program Highlights

- Two plenary sessions with lectures of four SCS prize winners 2024
- Nine thematic parallel sessions with keynote lectures and 15min PhD presentations
- Poster session during the lunch break
- Best oral and best poster presentation award ceremony
- Commercial exhibition

Topics of the Parallel Sessions

- Analytical Sciences
- Catalysis Science & Engineering
- Computational Chemistry
- Chemistry and the Environment
- Inorganic & Coordination Chemistry
- Medicinal Chemistry & Chemical Biology
- Organic Chemistry
- Physical Chemistry
- Materials Chemistry



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UNIVERSITÉ DE FRIBOURG
UNIVERSITÄT FREIBURG

WELCOME TO THE 2024 FALL MEETING OF THE SWISS CHEMICAL SOCIETY (SCS)



Prof. Ali Coskun



Hans Peter Lüthi

On behalf of the Organizing Committee, the Members of the Boards of all participating SCS Networks, the Department of Chemistry of the University of Fribourg and the Haute école d'ingénierie et d'architecture Fribourg HEIA, we welcome you to the SCS Fall Meeting 2024!

This is the first time that the Fall Meeting will be organized in Fribourg and it will be held at the Perolles Campus of the University, a wonderful venue for the Fall Meeting. The meeting will be a one-day event full of exciting science and will follow the traditional Fall Meeting format. After the welcome and opening, we will enjoy the award lectures, followed by nine thematic parallel sessions, which will serve as platforms for researchers to share their research findings. During the lunch break, the participants will have the opportunity to visit the poster session and the commercial exhibition. In the afternoon session, there is the second round of parallel sessions and award lectures. The meeting will be concluded with the announcement of the winners of the Helvetica prize and the award ceremony, honoring the best oral and poster presenters.

Introduced over twenty years ago, the Best Presentation Award Ceremony has become one of the highlights of the Fall Meeting. It marks the last item on the program of an intensive one-day conference. For more than a decade, Metrohm (oral presentations) and dsm-firmenich (posters) have been sponsoring this outstanding and very generous award program. With the first prizes in the best poster and the best oral presentation categories of each parallel session, in addition to cash and travel-awards, there is also the invitation to contribute to the Junior Laureates issue of *CHIMIA* published in April. For more details on the Award Program, please visit the respective section of the Fall Meeting website. Given the large number of presentations and the limited time available for the juries, the selection process, certainly for the poster contributions, is not an easy task. The attribute 'best' should therefore not be taken literally, but it is fair to say that the presentations of the winners will be of outstanding quality. We wish you the best of luck when presenting your research!

The Fall Meeting provides a unique platform for scientists, researchers, and industry professionals to share their latest findings, exchange ideas, and foster collaborations to drive future advancements. We are excited to host more than 400 researchers who will cover a wide range of topics. Overall, the presentations of senior lecturers included, there will be 114 oral presentations. At the poster session, 317 posters will be presented, creating a wonderful environment for scientific exchange and stimulating discussions between the participants.

We gratefully acknowledge the generous support from our sponsors, many of whom have been with us for a long time. We thank all the members of the organizing committee for curating an engaging and insightful session program. We invite you to review the program and look forward to meeting you in Fribourg!

Prof. Ali Coskun
Chairman of the
Organizing Committee

Hans Peter Lüthi
Director of the SCS Foundation

PROGRAM OVERVIEW, THURSDAY, 5TH SEPTEMBER 2024

The complete program incl. abstracts of all lectures, talks and posters are published on <https://fm24.scg.ch>

Time	Program Item
09.15	Welcome and conference opening Prof. Ali Coskun , University of Fribourg Chair of the SCS Fall Meeting 2024
Morning Plenary Session (Award Lectures) - Chair Prof. Christian Bochet, SCS President	
09.30	Werner Award Lecture 2024 Prof. Athina Anastasaki , ETH Zurich «Monomers from Polymer»
10.00	Sandmeyer Award Lecture 2024 The Eawag team "Advanced wastewater treatment" , Eawag/EPFL Lausanne Speakers: Prof. Urs von Gunten, Dr. Christa S. McArdell «Advanced wastewater treatment by ozonation for abatement of micropollutants from municipal wastewater effluents»
10.30	Short Break Relocation to the lecture halls of the parallel sessions
Morning Parallel Sessions	
10.45	Invited Lecture (30min) and Short Talks (15min) Topics: Analytical Sciences, Catalysis Science & Engineering, Computational Chemistry, Chemistry and the Environment, Inorganic & Coordination Chemistry, Medicinal Chemistry & Chemical Biology, Organic Chemistry, Physical Chemistry and Materials Chemistry
Lunch Break	
12.30	Poster Sessions (same topics as the parallel lecture sessions) Commercial Exhibition Visit the booths and inform yourself about the latest developments of our partners Participate in the exhibitor quiz and get the chance to win 1x 100 CHF and 2x 50 CHF in cash.
13.30	General Assembly of the youngSCS 2024 Lead: Marie-Désirée Schlemper-Scheidt, President youngSCS
Afternoon Parallel Sessions	
14.30	Invited/Sponsored Lecture (30min) and Short Talks (15min) Topics: Analytical Sciences, Catalysis Science & Engineering, Computational Chemistry, Chemistry and the Environment, Inorganic & Coordination Chemistry, Medicinal Chemistry & Chemical Biology, Organic Chemistry, Physical Chemistry and Materials Chemistry
16.15	Short Break Relocation to the lecture hall Joseph Deiss or the big lecture hall at HEIA-FR (streaming)
Afternoon Plenary Session (Award Lectures) - Chair Prof. Christian Bochet, SCS President	
16.30	Green & Sustainable Chemistry Award Lecture 2023 (sponsored by Syngenta) Prof. Ali Coskun , University of Fribourg «Porous Materials for Energy and Environmental Applications»
17.00	SCS Industrial Science Award Lecture 2024 Dr. Rosa Maria Rodriguez Sarmiento , F. Hoffmann-La Roche Ltd «Small Molecules Gamma Secretase Modulators for the treatment of Alzheimer's Disease»
SCS Announcements and Ceremony Session	
17.45	SCS Announcements Helvetica Prize of the Swiss Chemical Society 2024 David Spichiger, Richard Smith, Eva Hevia, Jérôme Waser
18.00	Best Oral Presentation Awards (sponsored by Metrohm) Markus Steinke, Marketing Manager at Metrohm International Headquarters Best Poster Presentation Awards (sponsored by dsm-firmenich) Jonathan Medlock, Principal Scientist EMEA, dsm-firmenich.
18.30	End of the conference
18.45	General Assembly of the youngSCS

GENERAL INFORMATION

Date: September 5, 2024, 08.30–18.30h
 Location: Campus Pérolles, University of Fribourg
 And HEIA Fribourg
 Host: University of Fribourg
 Website: <https://fm24.scg.ch/>

Conference Secretariat

Swiss Chemical Society
 David Spichiger, Céline Wittwer and Sarah Schmitz
 Haus der Akademien
 Laupenstrasse 7, Postfach
 3001 Bern
info@scg.ch

Organizing Committee

Chairmen

Prof. Ali Coskun, University of Fribourg
ali.coskun@unifr.ch
 Dr. Hans Peter Lüthi, SCS Foundation
luethi@scg.ch

Local Supporters

Ms. Maja Ivanovic, University of Fribourg
 Prof. Olivier Nicolet, HEIA-FR

Session Chairs

Analytical Sciences
 – Dr. Ralf Kaegi, Eawag Dübendorf
 – Prof. Chan Cao, University of Geneva

Catalysis Sciences & Engineering

– Prof. Martin Albrecht, University of Bern
 – Dr. Vladimir Paunovic, ETH Zurich
 – Dr. Cecilia Mondelli, Sulzer

Computational Chemistry

– Prof. Sandra Lubner, University of Zurich
 – Prof. Kjell Jorner, ETH Zurich

Inorganic & Coordination Chemistry

– Prof. Murielle Delley, University of Basel
 – Prof. Ross Milton, University of Geneva

Organic Chemistry

– Prof. Francesca Paradisi, University of Bern
 – Prof. Michal Juricek, University of Zurich

Medicinal Chemistry & Chemical Biology

– Prof. Fides Benfatti, University of Bern
 – Prof. Dennis Gillingham, University of Basel

Physical Chemistry

– Prof. Malte Oppermann, University of Basel
 – Prof. Natalie Banerji, University of Basel

Materials Chemistry

– Prof. Fabian von Rohr, University of Geneva
 – Prof. Bastian Brand, ZHAW Wädenswil

Chemistry and the Environment

– Dr. Thomas Bucheli, Thomas Bucheli GmbH
 – Dr. Jutta Hellstern, F. Hoffmann-La Roche Ltd

Registration

Fees for presenters (poster or talk)

– SCS Members: free of charge (by convention the first name in the abstract author list).

– Non-members: CHF 250.00 (incl. VAT).

Fees for participants without a presentation

– SCS Members: free of charge. However, registration is mandatory.

– Non-members: CHF 100.00 (incl. VAT).

Pre-registered participants will get an invoice in advance to avoid waiting time at the check-in desk. Participants who register after August 18 will have to pay the fees by credit card during the registration process.

If attending as a SCS member you have to bring your SCS membership-card with you! To become a member, please apply on <https://scg.ch/membership>.



Program and Abstract Search

The website allows you an easy and interactive planning of your conference day. Profit from the following functions:

- Interactive program overview with abstract preview
- Quick abstracts display as html file
- pdf-file download of single abstracts
- Extensive search functionalities



Schedule of SCS Fall Meeting 2023

Select Topic: Inorganic & Coordination Chemistry

Please Select Conference Day: 25 Aug 2023

Start Time	Inorganic & Coordination Chemistry	CC
08:30	Registration, Check-In, Welcome Coffee → SCS Fall Meeting 2023, Swiss Chemical Society (SCS)	
09:30	Generating Spin-Triplets at the Perovskite/Organic Interface Leo Niehous, Florida State University	
10:00	Small Molecules Targeting the Endocannabinoid System Uwe Grether, F. Hoffmann-La Roche AG	
10:30	Short Break (15min) → SCS Fall Meeting 2023, Swiss Chemical Society (SCS)	
10:45	Rationally Designed Long-Wavelength-Absorbing Metal Complexes as Photosensitizers for Photodynamic Therapy Giles Gosse, CHIRP-Tech, PSL University	
11:15	Synthesis and Reactivity of a Stable Organometallic Complex and Its Relevance to C-H Bond Activation Wojciech Stroh, University of Bern	
11:30	Behavior of (silver) ion binding with peptides exposed from SFE proteins Alexander Blansch, University of Fribourg	
11:45	Orientational self-sorting in octahedral palladium cages: scope and limitations of the cis rule Jeanne Mortierlin, EPFL Lausanne	
12:00	Surface Morphology and Interfacial Electric Fields of Inorganic Materials Tao-Chin Chia-Chang Chen, Universitat Basel	
12:15	⁵¹ NMR Anisotropy on Transition Metal (irido) Complexes: Link between Spectroscopy and Reactivity Yuya Kakuchi, ETH Zurich	
12:30	Lunch, Poster Session, Exhibition and Career Center	

Conference Framework: Building 08

4 Inorganic & Coordination Chemistry, Short talk
Synthesis and Reactivity of a Stable Organometallic Complex and its Relevance to C-H Bond Activation
 W. Stroh¹, M. Kubacki¹, L. A. Malague¹, S. Gudwin¹, K. Meyer², M. Albrecht³
¹Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, ²Department of Chemistry & Pharmacy, Inorganic Chemistry, Friedrich-Alexander-University Erlangen-Nürnberg
 The formation of C-N bonds is of paramount importance for synthesis of pharmaceuticals, agrochemicals and natural products.¹ Complexes with organo-oxides are critical precursors for the formation of strong covalent bonds to the inert C-H activation, forming C-N bonds very efficiently and sustainably. Despite their relevance, these rare transition metals with organo-oxides combined are extremely rare^{2,3} and they have been observed so far only, even though incorporation can be the first metal-oxido C-H activation analysis in organo-oxides.⁴

In this contribution we will show the first example of the full characterization of such an organometallic complex. We will demonstrate the further reactivity to a transient nitrene intermediate and discuss reactivity of the stable both in solution and in crystals. The characterization of both these intermediates is of paramount importance for understanding the catalytic C-H activation reactions and for designing new and improved catalytic systems.

[1] W. Stroh, J. Am. Chem. Soc., **2019**, *141*, 2141-2147
 [2] W. Stroh, M. Kubacki, M. H. L. Cantel, P. J. Chubb, D. J. M. Smith, *Angew. Chem.*, **2018**, *130*, 7997-8002
 [3] H. Wang, H. B. Aronoff, D. S. Shao-Liang, Z. Zhang, J. H. Reibman, D. C. Frazier, T. D. Swales, *J. Am. Chem. Soc.*, **2018**, *140*, 11122-11124
 [4] W. Stroh, M. Kubacki, M. H. L. Cantel, M. P. P. F. Gomes, M. Albrecht, *J. Am. Chem. Soc.*, **2013**, *135*, 21917-21918
 [5] W. Stroh, J. Am. Chem. Soc., **2013**, *135*, 951-962
 [6] W. Stroh, M. Albrecht, *Chem. Sci.*, **2013**, *4*, 2449-2459

Coffee Breaks and Lunch

Complementary refreshments will be served before the opening ceremony and during the breaks. Sandwiches/wraps and drinks will be served during the lunch break.

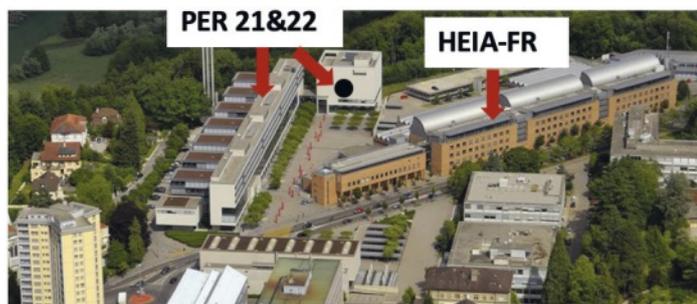
There is the option to buy lunch at your own expense at the cafeterias and restaurants located in the vicinity of the meeting venue.

Connection to the Internet

A wireless LAN (Wi-Fi) offers you access to the internet. Members of institutions participating to the Switch-Mobile project (all Swiss universities) will be able to connect by simply using their usual VPN client software. Other users will have to register first through a secure web page or can use the Swisscom Hotspot.

CONFERENCE VENUE

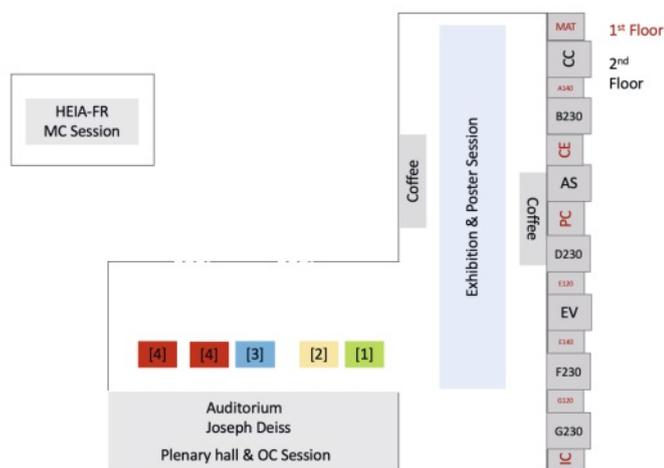
How to get to the Campus Péroles (PER 21 & 22)
Bd de Péroles 90, 1700 Fribourg



Public transport

SBB railway schedule on <https://sbb.ch>.

By train: from Fribourg railway station take the Bus 10/1/8/9 to the "Fribourg, Plateau des Péroles" stop, then a two-minute walk.



Registration Process

- 1 SCS members with member card
Registered participants with conference badge
- 2 Invited speakers, guests
Session chairs, jury members
- 3 SCS members without member card
- 4 Non-pre-registered participants
Non-SCS members
Onsite registration as SCS member

Rooms for Parallel Sessions

Plenary lectures: Joseph Deiss auditorium (002)
Organic Chemistry: Joseph Deiss auditorium (002)
Medicinal Chemistry: HEIA-FR big auditorium
Inorganic Chemistry: G 140
Computational Chemistry: C 120
Catalysis Sciences & Engineering: C 140
Physical Chemistry: A 120
Analytical Sciences: E 120
Materials Chemistry: G 120
Environmental Chemistry: E 140

Abstract codes

AS Analytical Sciences
CE Catalysis Sciences & Engineering
CC Computational & Theoretical Chemistry
EV Chemistry and the Environment
IC Inorganic Chemistry
MC Medicinal Chemistry & Chemical Biology
OC Organic Chemistry
PC Physical Chemistry
Mat Materials Chemistry

[XY-001]...[XY-027] Oral Presentations
[XY-101]...[XY-199] Posters

Department of Chemistry, University of Fribourg

<https://www.unifr.ch/chem/>



The Department of Chemistry at the University of Fribourg engages in modern areas of scientific research with a strong emphasis on soft matter and nanomaterial research. The Chemistry Department at Fribourg University proud to own analytical and synthetic research facilities of the highest international standards. There are numerous collaborations as well as researchers from all over the world that create an international and diverse working environment in our department. Several recent new hires make our department one of the youngest and most dynamic in the country. Excellent research facilities and expertise in modern areas of research enable an efficient and enjoyable teaching environment at the bachelor, master and doctorate level.

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

School of Engineering and Architecture of Fribourg

<https://www.heia-fr.ch>



Fribourg has a long history of professional education dating back to 1896, when the first vocational school opened with a class of 12 apprentice mechanics and stonecutters. Almost 120 years later, in 2015, the 1'000- student milestone was reached for the first time.

The HEIA-FR is a renowned and dynamic center for higher professional education and training, as evidenced by the steady growth of its student body. Its departments address the technological challenges of the future.

In addition to its teaching mission, the HEIA-FR hosts a rich applied research and development (aR&D) network with close ties to the economy: the institutes and centers of competence address the technical and scientific challenges defined by their numerous regional and national partners.

BEST PRESENTATION AWARDS

The organizers are proud of the very attractive presentation award program in which all presenters automatically participate. More than CHF 42'000 CHF in total are given to the winners in monetary form, travel grant or free publication opportunities in the Junior Laureates issue of CHIMIA 4/2025.

We like to address our recognition and thank to the Metrohm Foundation and to dsm-firmenich, that are partnering for the presentation award program for many years.



Best Oral Presentation Award

The award is sponsored by Metrohm.

The prize is given for the two best short presentations of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 05.09.2024, 18.10h in the auditorium Joseph Deiss.

Prize for the winner of each of the nine, parallel sessions

- Cash contribution of CHF 500
- Travel voucher of CHF 1'000 to attend an international conference.
- Invitation to present the research in the laureates' issue of CHIMIA. Value CHF 1'200.

Prize for the Runners-up

- Cash contribution of CHF 400.

The prizes are sponsored by Metrohm and will be handed over by Dipl. Ing. Markus Steinke, Executive Vice President Marketing at Metrohm International Headquarters, Herisau

HELVETICA PRIZE OF THE SWISS CHEMICAL SOCIETY 2024



Helvetica and the Swiss Chemical Society are proud to award the 2024 winners of the Helvetica Prize of the Swiss Chemical Society for the best published papers of PhD/Postdocs 2023/24 in Helvetica Chimica Acta. The prize is endowed with CHF 1'000 for the winner and CHF 500 for the runner up. The prize was implemented in 2019 to honor outstanding publications of young researchers in Switzerland.

Richard Smith, Executive Editor of Wiley-VHCA will honor the winners.

Covers of the 2022–2024 Junior Laureates Issues



Best Poster Presentation Award

The award is sponsored by dsm-firmenich.

The prizes were given for the best posters/short video of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 05.09.2024, 18.20h in the auditorium Joseph Deiss.

Prize for the winner of each of the seven, poster session

- Cash contribution of CHF 200.
- Travel voucher of CHF 750 to attend an international conference.
- Invitation to present the research in the laureates' issue of CHIMIA. Value CHF 1'200.

Prizes for the Runners-up

- 1–2× cash contributions of CHF 200.

The prizes are sponsored by dsm-firmenich and will be handed over by Dr. Jonathan Medlock, Principal Scientist EMEA, dsm-firmenich.

EXHIBITOR CHALLENGE

Visit our exhibition and participate in the exhibitor challenge.



Full cards with stickers from all our partners take part in the lucky draw of 1×100.00 CHF. Cards with at least one full column or one full row take part in the draw of 2× 50.00 CHF.

The prize draw takes place on September 5, at 17:45h.

SPONSORS AND SUPPORTERS

The SCS and the meeting organizers gratefully acknowledge the generous support of its main sponsors, session sponsors and exhibitors. Without their contributions, it would not be possible to organize this event on an annual basis.

SCS MAIN SPONSORS AND GENERAL SUPPORTERS



European Chemical Societies Publishing



ENDOWMENTS OF PARALLEL SESSIONS



Analytical Sciences



Catalysis Science & Engineering



Computational Chemistry



Chemistry and the Environment



Inorganic & Coordination Chemistry



Medicinal Chemistry & Chemical Biology



Organic Chemistry



Physical Chemistry



Materials Chemistry

COMMERCIAL EXHIBITORS



Award Lectures Plenary Sessions

Werner Prize 2024

«Monomers from Polymer»

September 5, 2024, 09.30–10.00h

Prof. Athina Anastasaki, ETH Zurich, received the prize for her excellence in research spanning across the broad areas of polymer synthesis, polymer self-assembly and chemical recycling, also referred to as depolymerization.



Sandmeyer Award 2024

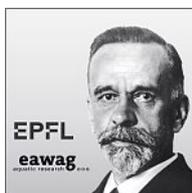
«Advanced wastewater treatment by ozonation for abatement of micropollutants from municipal wastewater effluents»

September 5, 2024, 10.00–10.30h

Speakers: Urs von Gunten, Christa S. McArdell

The Eawag team “Advanced wastewater treatment”, namely Prof. Urs von Gunten, EPFL Lausanne/Eawag, Prof. Juliane Hollender, ETH Zurich, Dr. Christa McArdell, Dr. Adriano Joss, Marc Böhler and Dr. Christian Abegglen, Eawag, and Prof. em. Hansruedi Siegrist, ETH Zurich,

is awarded in recognition of the team’s outstanding achievements in using chemistry to address a challenge of large societal importance: securing clean water.



Green & Sustainable Chemistry Award 2023

«Porous Materials for Energy and Environmental Applications»

September 5, 2024, 16.30–17.00h

Prof. Ali Coskun, University of Fribourg, received the prize for his outstanding contributions towards the development of sustainable polymers for catalysis, energy and environmental applications.



SCS Industrial Science Award 2024

«Small Molecules Gamma Secretase Modulators for the treatment of Alzheimer’s Disease»

September 5, 2024, 17.00–17.30h

Dr. Rosa Maria Rodriguez Sarmiento,

F. Hoffmann-La Roche Ltd,

is awarded for her impactful contributions to numerous research initiatives in various therapeutic areas such as CNS and rare diseases, as well as cardiovascular and metabolic diseases coupled with her influence on the scientific community both within and outside the company.



THEMATIC PARALLEL SESSIONS

Analytical Sciences [AS]
Morning Session – PER 21, E120



Chair: Ralf Kaegi, Eawag

Session Endowment: Metrohm

- 10:45 **Highest precision radiocarbon measurements for accurate dating and tracer studies [AS-011]**
Lukas Wacker, ETH Zurich
- 11:15 **The central role of oxo clusters in zirconium and hafnium-based esterification catalysis. [AS-013]**
Jikson Mathew, University of Basel
C. Seno, M. Jaiswal, C. Simms, N. Reichholf, D. Van den Eynden, T. Parac-Vogt, J. De Roo*
- 11:30 **Retrospective Verification of Exposure of Human Blood Serum to Sesquimustard via Semi-Targeted Proteomic Analysis [AS-014]**
Gianin Thomann, Spiez Laboratory/University of Fribourg
M. Brackmann, C. G. Bochet, C. Curty*
- 11:45 **Oxygen Isotope Analyses of Phosphate and Organophosphorus Compounds by Orbitrap High-Resolution Mass Spectrometry [AS-015]**
Nora Bernet, Eawag / ETH Zurich
F. Tamburini, T. B. Hofstetter*
- 12:00 **Conformational Analysis with High-Resolution mid-IR Laser Absorption Spectroscopy [AS-016]**
Miloš Selaković, Empa
L. Emmenegger, R. Zenobi, B. Tuzson*
- 12:15 **OctoChemDB: A Web Service for Efficient Dereplication of Natural Products using High-Resolution Mass Spectra [AS-017]**
Ricardo Silvestre, HEIA Fribourg
R. Martinent, V. Mutel, C. Portmann, L. Menin, L. Patiny

Afternoon Session – PER 21, E120

Chair: Chan Cao, University of Geneva

- 14:30 **Mitigating Bottlenecks in NIR Model Development [AS-021]**
Christoph Jansen, Metrohm Switzerland
- 15:00 **Label free identification of full-length proteins and protein modifications using a nanopore [AS-023]**
Verena Rukes, EPFL Lausanne
E. Norkute, G. Barnikol, J. Gao, C. Cao*
- 15:15 **Quantification of laser generated aerosols via microdroplet calibration using a downwards pointing ICP-TOFMS [AS-024]**
Tobias Schöberl, ETH Zurich
M. Bachmann, D. Günther*
- 15:30 **The potential of ultra-trace lanthanide impurities in nuclear forensic evidence [AS-025]**
Michael Hofstetter, ETH Zurich
S. Röllin, P. Steinegger
- 15:45 **Detection of nanoplastics using SERS tags at environmentally relevant concentrations [AS-026]**
Moritz Häffner, Adolphe Merkle Institute, Fribourg
B. Rothen-Rutishauser, P. Taladriz-Blanco, A. Perti-Fink*
- 16:00 **Capacitive displays as direct signal transducers for potentiometric measurements [AS-027]**
Yaotian Wu, University of Geneva
E. Bakker*

Catalysis Sciences & Engineering [CE]
Morning Session – PER 21, C140
 Chair: Vladimir Paunovic, ETH Zurich



- Session Endowment: Carbogen Amcis
- 10:45 **Minimalistic Models of Oxotransferases as Catalysts for Site and Enantioselective Oxidation of Strong C-H Bonds [CE-011]**
 Miquel Costas, Universitat de Girona
- 11:15 **Developemnt of a self-optimizing platform for flow-based peptide synthesis [CE-013]**
 Bálint Tamás, University of Zurich
 P. L. Willi, H. Bürgisser, N. Hartrampf*
- 11:30 **Tracking Active Site Formation in Cu-Exchanged Zeolites for Partial CH₄ Oxidation [CE-014]**
 Andreas Brenig, ETH Zurich/PSI
 J. W. Fischer, D. Klose, G. Jeschke, J. A. van Bokhoven*, V. L. Sushkevich*
- 11:45 **CO₂ electroreduction to long-chain hydrocarbons on cobalt catalysts [CE-015]**
 Phil Preikschas, ETH Zurich
 J. Zhang, R. R. Seemakurthi, Z. Lian, A. J. Martín, S. Xi, N. López, B. Yeo, J. Pérez-Ramírez*
- 12:00 **Decoding the Promotional Effect of Iron in Bimetallic Pt-Fe-Nanoparticles for the Low Temperature Reverse Water-Gas Shift Reaction [CE-016]**
 Colin Hansen, ETH Zurich; W. Zhou, C. Copéret*
- 12:15 **Accelerating transfer hydrogenation of sterically hindered ketones with a novel mono-substituted amino-carbene (MAC) ruthenium complex [CE-017]**
 Giacomo Rigoni, University of Bern
 M. Casciotti, T. Belderrain, P. Pérez*, M. Albrecht*

Afternoon Session – PER 21, C140
 Chair: Cecilia Mondelli, Sulzer

- 14:30 **First Industrial (Total) Synthesis of Amanitin Derivatives [CE-021]**
 Emad El Sayed, Carbogen Amcis AG
 A. Krotz, K. Williams, L. Shapely, P. Brown, J. Bowen, I. Sulaiman, E. Lauterbach, J. Kovacs, S. Ruppenthal, B. Vivant, L. Mannocci, M. Doll, A. Osypenko, W. Simon, C. Lutz, C. Müller
- 15:00 **Operando XAS-XRD Reveals Structural Dynamics in CoPt Nanoparticles under Dry Reforming of Methane Conditions [CE-023]**
 David Niedbalka, ETH Zurich
 M. Janak, D. Piankova, N. Zimmerli, P. M. Abdala, C. R. Müller*
- 15:15 **Engineering a Dual-Functionalized PolyHIPE Resin for Photobiocatalytic Flow Chemistry [CE-024]**
 Emmanouil Broumidis, University of Bern
 F. Paradisi*
- 15:30 **Ruthenium-NHC complexes as precursors for highly active lignin hydrogenolysis catalysts [CE-025]**
 Lindsey Frederiksen, EPFL Lausanne
 P. Dyson*
- 15:45 **Multi-origin and topology-dependent selectivity in the methanol-to-olefins process from transient operando DRIFTS-GC [CE-026]**
 Luca Maggiulli, PSI
 J. A. Van Bokhoven, D. Ferri*
- 16:00 **Design and Characterisation of a de novo Gold Artificial Metalloenzyme [CE-027]**
 Elinor Morris, University of Basel
 J. Uhrhan, B. Lozhkin, S. Basler, I. Kalvet, T. R. Ward*, D. Baker*

Computational Chemistry [CC]
Morning Session – PER 21, C120
 Chair: Sandra Luber, University of Zurich



- Session Endowment: Johnson&Johnson Innovative Medicine
- 10:45 **Simulating non-adiabatic dynamics in molecules: methodological aspects and attochemical applications [CC-011]**
 Morgane Vacher, Nantes Université
- 11:15 **From capture to catalysis: Insights from atomistic simulations into MOF and COF host-guest interactions and guest dynamics [CC-013]**
 Michelle Ernst, University of Zurich
 J. Hutter*
- 11:30 **Unravelling Tunnelling Effects in Photosensitization using Instanton Theory [CC-014]**
 Meghna Manae, ETH Zurich
 J. Richardson*
- 11:45 **Ab initio simulation of single vibronic level fluorescence spectra using Hagedorn wavepacket [CC-015]**
 Zhan Tong Zhang, EPFL Lausanne
 J. Vanicek*
- 12:00 **Accelerating Alchemical Free-Energy Calculation with the RE-EDS Multistate Method [CC-016]**
 Candide Champion, ETH Zurich
 R. Gall, B. Ries, S. Rieder, E. Pécora de Barros, P. Hünenberger*, S. Riniker*
- 12:15 **Automated Chemical Reaction Network Exploration of Oxidative Water Treatment [CC-017]**
 Enric Petrus, Eawag, Dübendorf
 U. von Gunten, M. Reiher, T. B. Hofstetter*

Afternoon Session – PER 21, C120
 Chair: Kjell Jorner, ETH Zurich

- 14:30 **Computational approaches in pharma on chemical reactivity and affinity optimization [CC-021]**
 Herman Van Vlijmen, Johnson & Johnson Innovative Medicine R&D
- 15:00 **Applying a well-defined energy density for machine-learned density functionals [CC-023]**
 Elias Polak, University of Fribourg
 S. Vuckovic, H. Zhao
- 15:15 **Inverse Design of Singlet Fission Materials with Uncertainty-Controlled Genetic Optimization [CC-024]**
 Luca Schaufelberger, ETH Zurich
 R. Laplaza, J. T. Blaskovits, C. Corminboeuf*, K. Jorner*
- 15:30 **Saturn: Sample-efficient Generative Molecular Design using Memory Manipulation [CC-025]**
 Jeff Guo, EPFL Lausanne
 P. Schwaller*
- 15:45 **A Metadynamics Study of Water Oxidation Reactions at (001)-WO₃/liquid-water Interface [CC-026]**
 Rangsiman Ketkaew, University of Zurich
 F. Creazzo, K. Sivula, S. Luber*
- 16:00 **Global and Local Electrophilicity as Measure of Endocrine Disruptor Genotoxicity Potential [CC-027]**
 Sophia Johnson, EPFL Lausanne
 S. Guilbert, U. Rothlisberger*

Chemistry and the Environment [EV] **Morning Session – PER 21, E140**

Chair: Thomas Bucheli, Thomas Bucheli GmbH

Session Endowment: Casale SA

- 10:45 **Chemistry Hacks: Tweaking Air Composition to Tackle Respiratory Virus Transmission [EV-011]**
Tamar Kohn, EPFL Lausanne
- 11:15 **Effect of surfactants on inactivation of *Bacillus subtilis* spores by chlorine [EV-013]**
Tianqi Zhang, EPFL Lausanne
M. I. Villalba, R. Gao, S. Kasas, U. von Gunten*
- 11:30 **In search of alternative herbicides to treat Swiss railway tracks [EV-014]**
Valérian Zeender, Agroscope
R. Kasteel, T. Poiger, I. Buerge
- 11:45 **Mining Actinomycetes' Metabolomes and Genomes for Anti-*Phytophthora infestans* Compounds [EV-015]**
Ola Abdelrahman, University of Fribourg
Q. Coxon, E. Abou-Mansour, F. L'Haridon, L. Falquet, P. Allard, L. Weisskopf*
- 12:00 **Organic micropollutants in combined sewer overflows challenge sustainable water management [EV-016]**
Viviane Furrer, Eawag, Dübendorf
C. Ort, H. Singer, C. Ort*, H. Singer*
- 12:15 **Preserving the Biotransformation Potential of Activated Sludge in Time: Towards Reproducible Incubation Experiments for Persistence Assessment [EV-017]**
Martina Kalt, Eawag, Dübendorf
C. Udressy, Y. Yu, A. Colliquet, K. Fenner*

Afternoon Session – PER 21, E140

Chair: Jutta Hellstern, Roche

- 14:30 **Environmental chemistry for a sustainable future [EV-021]**
Pierdomenico Biasi, Casale SA
- 15:00 **Biochars from chlorine-rich feedstock are low in polychlorinated dibenzo-*p*-dioxins, -furans and -biphenyls [EV-023]**
Jannis Grafmüller, Ithaka Institut
D. Rathnayake, N. Hagemann, T. Bucheli, H. Schmidt
- 15:15 **Differentiating Olefins and Phenols using the Stable Oxygen Isotope Composition of H₂O₂ Formed during Ozonation [EV-024]**
Seok Kim, Eawag, Dübendorf
T. B. Hofstetter, U. v. Gunten*
- 15:30 **Indirect aquatic photolysis of polyethylene glycol influences the biodegradability in soil and sediment: Linking kinetic simulations to experimental observations [EV-025]**
Kevin Kleemann, ETH Zurich
M. Sander*
- 15:45 **Extracellular Electron Transfer in *Geobacter Sulfurreducens* [EV-026]**
Salem Majouri, University of Fribourg
B. Giese, K. M. Fromm*
- 16:00 **Comparative Study of Chelating Agents in the Treatment of Heavy Metal Poisoning on Early Zebrafish Embryo Development [EV-027]**
Dib Chakif, University of Bern
A. Elhelbawi, J. Imhof, I. Gjurroski, S. Leidel*, J. Furrer*

Inorganic & Coordination Chemistry [IC] **Morning Session – PER 21, G140**

Chair: Murielle Delley, University of Basel

Session Endowment: Chemspeed

- 10:45 **Inspired by Nitrogenase: Dihydride Complexes for the H₂-Releasing Reductive Activation of Challenging Substrates [IC-011]**
Franc Meyer, University of Göttingen
- 11:15 **Nano onions based on an amphiphilic gold(I) cyclic trinuclear complex [IC-013]**
Atena B. Solea, EPFL Lausanne
D. Dermutas, F. Fadaei Tirani, K. Severin*
- 11:30 **Symmetry and Rigidity for Boosting Erbium-Based Molecular Light-Upconversion in Solution [IC-014]**
Ines Taarit, University of Geneva
S. Naseri, C. Piguet*
- 11:45 **Gold(III)-hydrides stabilized by novel (P[^]N[^]C) pincer ligands [IC-015]**
Jaime Martín, University of Zurich
C. Nevado*
- 12:00 **Cyclopentadienone Iron Complex-Catalyzed Hydrogenation of Ketones: The Influence of the Charge-Tag on Catalytic Performance [IC-016]**
André Bütikofer, ETH Zurich
V. Kesselring, P. Chen*
- 12:15 **Non-classical azolyidene metal complexes as potential anticancer therapeutics [IC-017]**
Jan Romano-deGea, EPFL Lausanne
P. J. Dyson*

Afternoon Session – PER 21, G140

Chair: Ross Milton, University of Geneva

- 14:30 **Enhancing Energy Research [IC-021]**
Ahmed Mahmoud, Chemspeed
- 15:00 **The Influence of an ortho-methyl Group in Rhodium-PYA Complex Reactivity and Catalysis [IC-023]**
Llorenç Benavent Benavent, University of Bern
J. Race, L. Studer, M. Albrecht*
- 15:15 **The Influence of SiO₂ Dehydroxylation on Offline Thermochromatography with ²⁰²Tl [IC-024]**
Jennifer Wilson, ETH Zurich/PSI
C. Gut, R. Eichler, N. P. van der Meulen, P. V. Grundler, P. Steinegger*
- 15:30 **Stabilization Effect of NH-S Hydrogen Bonds in Synthetic Iron-Sulfur and Iron-Selenium Clusters [IC-025]**
Alessandro Walker, ETH Zurich
M. Inoue, L. Grunwald, V. Mougél*
- 15:45 **Re-Evaluation of the Air-Mediated Response in Bi-Based Perovskite X-Ray Detectors [IC-026]**
Aditya Bhardwaj, ETH Zurich
K. Sakhatskyi, M. J. Gebhard, M. Kotyrba, S. Yakunin, M. Kovalenko*
- 16:00 **Tracking Ag⁺ ions from the SilE protein to the silver efflux pump in *E.coli* [IC-027]**
Chloé Morin-Payé, University of Fribourg
K. M. Fromm*

Medicinal Chemistry & Chemical Biology [MC]**Morning Session – HEIA**

Chair: Fides Benfatti, Syngenta

Lonza

Session Endowment: Lonza

- 10:45 **Engineered Protein Cages for RNA Delivery [MC-011]**
Angela Steinauer, EPFL Lausanne
P. Oeser, G. Barnikol, A. Melgar, A. Steinauer*
- 11:00 **Identification of a peripherally restricted MAGL inhibitor which shows promising activity in disease models of visceral pain and IBD [MC-012]**
Fionn O'Hara, F. Hoffmann-La Roche Ltd.
J. Benz, J. Blaising, U. Grether, M. Guerard, R. Koller, B. Kuhn, M. Reutlinger, W. Saal, M. Wittwer
- 11:15 **Expanding the Chemical Space of Lasso Peptides by Combining Flow Synthesis and Enzymatic Transformation [MC-013]**
Kevin Schiefelbein, University of Zurich
J. Lang, M. Schuster, C. E. Grigglesome, R. Striga, L. Bigler, M. C. Schuman, O. Zerbe, Y. Li, N. Hartrampf*
- 11:30 **Antimicrobial peptide-peptoid hybrids [MC-014]**
Etienne Bonvin, University of Bern; M. Orsi, J. Raymond*
- 11:45 **Two-for-One Biosynthesis: Functional Biosynthetic Stereodivergence in a Gene Cluster via a Dihydroxydnone N-oxide [MC-015]**
Jiajun Ren, University of Zurich
A. Mathew, M. Rodriguez Garcia, T. Kohler, O. Blacque, A. Linden, S. Sieber, L. Eberl*, K. Gademann*,
- 12:00 **Discovery of functional active low-molecular weight antagonists of IL-1B [MC-016]**
Anna Vulpetti, Novartis Pharma AG
- 12:15 **Local environment in biomolecular condensates modulates enzymatic activity across length scales [MC-017]**
Marcos Gil-Garcia, ETH Zurich; A. Benítez-Mateos, M. Papp, F. Stoffel, C. Morelli, K. Normak, K. Makasewicz, L. Faltova, F. Paradisi, P. Arosio*

Afternoon Session – HEIA, Big Lecture Hall

Chair: Dennis Gillingham; University of Basel

- 14:30 **Development and Manufacture of highly potent products at Lonza Visp Development Services [MC-021]**
Elisa González-Fernández, Lonza
- 14:45 **Semi-synthetic nucleosomes to probe sirtuin activity on chromatin [MC-022]**
Carlos Moreno Yruela, EPFL Lausanne; B. E. Ekundayo, E. Calviño Sanlés, D. Ni, H. Stahlberg, B. Fierz*
- 15:00 **A Far-Red Fluorescent Probe to Visualize Gram-Positive Bacteria in Patient Samples [MC-023]**
Krittvas Jantarug, University of Zurich
V. Tripathi, B. Morin, A. Lizuka, N. Khanna, D. Bumann, P. R. Fuentes*
- 15:15 **AI-Enabled Synthesis Prediction in Modern Medicinal Chemistry [MC-024]**
Kenneth Atz, F. Hoffmann-La Roche Ltd; D. F. Nippa, A. T. Müller, U. Grether, R. E. Martin, G. Schneider
- 15:45 **Discovery of NP3-562: a novel, orally bioavailable NLRP3-inhibitor [MC-026]**
Juraj Velcicky, Novartis Pharma AG; P. Janser, N. Gommermann, J. Dawson, K. Beltz, C. Dekker, C. J. Farady, A. Mackay

- 16:00 **Trabectedin derails transcription-coupled nucleotide excision repair to induce DNA breaks in highly transcribed genes [MC-027]**

Vakil Takhaveev, ETH Zurich; K. Son, V. Mor, H. Yu, E. Dillier, N. Zilio, N. J. Püllen, D. Ivanov, H. Ulrich, S. J. Sturla*, O. D. Schärer*

**Organic Chemistry [OC]
Morning Session – PER 22,
Joseph Deiss (002)**

Chair: Francesca Paradisi, University of Bern

syngenta.

Session Endowment: Syngenta

- 10:45 **Site-Selective Direct C–H Arylation [OC-011]**
Ilija Čorić, University of Zurich
- 11:15 **Radical-mediated azidofunctionalization of alkenes [OC-013]**
Pierre Palamini, EPFL Lausanne
E. M. Allouche, J. Waser*
- 11:30 **Photo- and Cobalt-Catalyzed Synthesis of Heterocycles via Cycloisomerization of Unactivated Olefins [OC-014]**
Willi Amberg, ETH Zurich
H. Lindner, T. Martini, D. M. Fischer, E. Moore, E. M. Carreira*
- 11:45 **Asymmetric, Remote C(sp³)-H Arylation via Sulfinyl-Smiles Rearrangement [OC-015]**
Yawen Hu, University of Zurich
C. Hervieu, E. Merino*, C. Nevado*
- 12:00 **Flow Chemistry for the Synthesis of the Anesthetic Mepivacaine, a More Sustainable Approach [OC-016]**
Pablo Díaz-Kruik, University of Bern
F. Paradisi*
- 12:15 **Total Synthesis of the Diterpenes (+)-Randainin D and (+)-Barekoxide via Photoredox-Catalyzed Deoxygenative Allylation [OC-017]**
Oleksandr Vyhivskiy, University of Basel
O. Baudoin*

Afternoon Session – PER 22, Joseph Deiss (002)

Chair: Michal Juricek, University of Zurich

- 14:30 **Enabling technologies at Syngenta: electrochemistry as a case study [OC-021]**
Andrei Iosub, Syngenta Crop Protection AG
M. Lehmann, C. Scarborough
- 15:00 **Vicinal Nucleophilic Disubstitution Reactions of (Densely Substituted) Arenes via 1,2-Bis-Triazenylarenes [OC-023]**
Christeena Mathew, EPFL Lausanne; K. Severin*
- 15:15 **Catalyst-stereocontrolled synthesis of alkyne atropisomers [OC-024]**
Lucía Reyes Méndez, University of Basel
D. Pepe, J. Dong, N. Sidler, D. Häussinger, C. Sparr*
- 15:30 **Electronic and Chiroptical Properties of Cations and Neutral Radicals of Enantiopure Diaza[4]helicenes [OC-025]**
Bibiana Fabri, University of Geneva
T. Funaioli, L. Frédéric, C. Elsner, E. Bordignon, F. Zinna, L. Di Bari, G. Pescitelli, J. Lacour*
- 15:45 **Photochromism in cyclic dipeptides: biocompatible switches and smart materials [OC-026]**
Zbigniew Pianowski, Karlsruhe Institute of Technology
Z. Pianowski*
- 16:00 **Synthesis of curved Polycyclic aromatic macrocycles towards shape-assisted self-assembly [OC-027]**
Ludmilla Sturm, University of Geneva; M. Rickhaus*

Physical Chemistry [PC]
Morning Session – PER 21, A120
 Chair: Malte Oppermann, University of Basel

METTLER TOLEDO

Session Endowment: Mettler Toledo

- 10:45 **Chiroptical probes to track spin & light polarization in space & time in emerging semiconductors [PC-011]**
 Sascha Feldmann, EPFL Lausanne
- 11:15 **Excited-State Symmetry Breaking and its Origins: Insights from Ultrafast Transient Two-Dimensional Infrared Spectroscopy [PC-013]**
 Ricardo Fernández-Terán, University of Geneva
 E. Balanikas, J. Kölbl, R. J. Fernández-Terán*, E. Vauthy*
- 11:30 **Real-time tracking of the ultrafast chirality and energy transfer in a chiral OLED complex with circularly-polarized luminescence [PC-014]**
 Livia Müller, University of Basel
 F. Zinna, G. Pescitelli, M. Puppini, M. Oppermann*
- 11:45 **Capturing site-selective chemical dynamics via time-resolved X-ray photoelectron spectroscopy [PC-015]**
 Andre Al Haddad, Paul Scherrer Institut PSI, Villigen
 S. Oberli, J. Knurr, L. Paoloni, A. Sarracini, K. Schnorr, A. Picon, C. Bostedt*
- 12:00 **Magnetic Deflection of Neutral Sodium Solvent Clusters: $\text{Na}(\text{H}_2\text{O})_n$, $\text{Na}(\text{NH}_3)_n$, $\text{Na}(\text{MeOH})_n$, and $\text{Na}(\text{DME})_n$ [PC-016]**
 D. Borgeaud dit Avocat, ETH Zurich
 J. V. Barnes, E. Simmen, B. L. Yoder, R. Signorell
- 12:15 **Competition between product channels in ion-molecule reactions near 0 K: $\text{D}_2^+ + \text{CH}_3\text{F}$ and $\text{D}_2^+ + \text{H}_2\text{O}$ [PC-017]**
 David Schlender, ETH Zurich; R. Hahn, F. Merkt*
- 12:30 5x 3min poster pitches

Afternoon Session – PER 21, A120
 Chair: Natalie Banerji, University of Bern

- 14:30 **Holographic Microscopy and Machine Learning – Transforming Cellular Assays [PC-021]**
 Natalia Jarzębska, Mettler Toledo GmbH
 A. Ferrer, H. Muhr*
- 15:00 **Multifunctional hybrid systems via self-organization of Janus nanoparticles and polymersomes for bio-applications [PC-023]**
 Voichita Mihali, University of Basel
 M. Skowicki, P. Jasko, C. Palivan*
- 15:15 **Innovative pH-Responsive Rhamnolipid Nanomaterials: Advanced Antimicrobial Solutions [PC-024]**
 Parth Kadakia, University of Fribourg
 J. Valentin, S. Salentinig*
- 15:30 **Rational Design of Dinitroxide Polarizing Agents for Dynamic Nuclear Polarization to Enhance Overall NMR Sensitivity [PC-025]**
 Ran Wei, EPFL Lausanne
 A. Venkatesh, G. Casano, Y. Rao, H. Lingua, H. Karoui, M. Yulikov, O. Ouari*, L. Emsley*
- 15:45 **Improved super-resolution imaging with cucurbituril-encapsulated fluorophores [PC-026]**
 Liza Briant, University of Geneva
 A. Fürstenberg*
- 16:00 **Insights into the Bonding Nature of Arsenic, Phosphorus, and Sulphur Ylides: an answer from quantum crystallography [PC-027]**
 Yaser Balmohammadi, University of Bern
 L. A. Malaspina, S. Grabowsky

Materials Chemistry [Mat]
Morning Session – PER 21, G120
 Chair: Fabian von Rohr, University of Geneva

Vigor

Session Endowment: Vigor

- 10:45 **Materials Chemistry and the Future of Human Civilization [Mat-011]**
 Nicola Spaldin, ETH Zurich
- 11:15 **End-functionalized high dielectric permittivity polysiloxanes for solvent-free processing [Mat-013]**
 Jana Wolf, EMPA
 P. M. Danner, J. von Szczepanski, D. M. Opris*
- 11:30 **A Dye-Sensitized Sensor for Oxygen Detection under Visible Light [Mat-014]**
 Lionel Wettstein, ETH Zurich
 J. Specht, V. Kesselring, L. Sieben, Y. Pan, D. Käch, F. Krumeich, D. Baster, M. El Kazzi, M. Bezdek*
- 11:45 **Supramolecular Modulation for Hybrid Perovskite Photovoltaics [Mat-015]**
 Ghewa AlSabeih, EPFL Lausanne / AMI
 M. Almalki, S. Kasemthaveechok, M. A. Ruiz-Preciado, P. Zimmermann, D. Dekker, M. Galerne, E. Moulin, F. T. Eickemeyer, M. Graetzel*, J. V. Milic*
- 12:00 **All-Perovskite Multicomponent Nanocrystal Superlattices [Mat-016]**
 Taras Sekh, ETH Zurich/Empha
 I. Cherniukh, G. Rainò, E. Kobiyama, T. Sheehan, W. A. Tisdale, T. Stöferle, R. Erni, G. Itkos, M. I. Bodnarchuk*, M. V. Kovalenko*
- 12:15 **hybrid hole-selective protection layer towards long-term stability of low-cost metal oxide in solar water oxidation [Mat-017]**
 Sanghyun Bae, University of Zurich
 D. Tilley*

Afternoon Session – PER 21, G120
 Chair: Bastian Brand, ZHAW Wädenswil

- 14:30 **Gloveboxes – Operation, Maintenance, and Common Misunderstandings [Mat-021]**
 Martin Eck, Vigor Gas Purification Technologies
- 15:00 **Epitaxial Core/Shell Nanocrystals of (Europium-Doped) zirconia and hafnia [Mat-023]**
 Carlotta Seno, University of Basel
 N. Reichholf, F. Salutari, M. Spadaro, Y. P. Ivanov, G. Divitini, A. Gogos, I. Herrmann, J. Arbiol, P. F. Smet, J. De Roo
- 15:15 **Tetraoxa[8]circulenes - A Platform for Polymers and Frameworks [Mat-024]**
 Patrick Fritz, University of Fribourg
 A. Coskun*
- 15:30 **Soft actuators based on stimuli-responsive composite hydrogels [Mat-025]**
 Matilde Folkesson, Adolphe Merkle Institute, Fribourg
 C. Weder*, J. A. Berrocal*
- 15:45 **Constructing Diverse Colloidal Suprastructures for Biomedical Advancements [Mat-026]**
 Minghan Hu, ETH Zurich
 S. Pané, B. Nelson, H. Thérien-Aubin, H. J. Butt, A. DeMello, L. Isa, M. Hu*
- 16:00 **Crystal growth and anisotropic magnetic properties of incommensurately modulated $\text{K}_{0.87}\text{CrSe}_2$ [Mat-027]**
 Felix Eder, University of Geneva
 C. Witteveen, J. F. Woods, R. Butti, P. Szwedziak, A. Vargas Jentzsch, M. Rickhaus, E. Giannini*, F. O. von Rohr*

SCS FALL MEETING 2024, POSTER SESSIONS**Poster Presentation Title [Code]**

First line = Presenting Author

Second line = Coauthors

Analytical Sciences [AS]**Poster Session****Mechanistic understanding of electric field enhancement in gap-mode tip-enhanced Raman spectroscopy [AS-101]**

Siiri Bienz, ETH Zurich

C. Hsu, K. Greis, R. Zenobi*, N. Kumar*

Mapping of surface functionality of (bio-based) polymers in relation to weathering (environmental decay) [AS-102]

Tobias Borgmeyer, EPFL Lausanne

M. J. Rossi, C. Ludwig*

Gas-phase fluorescence spectroscopy and ion mobility-mass spectrometry for investigating time-resolved unfolding mechanisms of cytochrome c after desolvation [AS-103]

Linus Busse, ETH Zurich

L. Benzenberg, R. Zenobi*

Combining NIR spectroscopy and chemometrics for the online determination of process temperature and spectra prediction [AS-104]

Federico Cambiè, PSI/EPFL Lausanne

I. Alxneit, D. Ferri, O. Kröcher

Automated Prediction of Ground State Spin for Transition Metal Complexes and Benchmarking Physics-based Representations [AS-105]

Yuri Cho, EPFL Lausanne

R. Laplaza, S. Vela, Y. C. Alonso, K. Briling, C. Corminboeuf*

A flow-electrolysis approach for the separation and analysis of plutonium [AS-106]

Paul Dutheil, Paul Scherrer Institute PSI, Villigen

F. Köhler, M. Heule*, P. Steinegger*

Examining the volatile organic compound profile of wild-type and gnotobiotic honey bees by high-resolution mass spectrometry [AS-107]

Mateusz Fido, ETH Zurich

S. Moriano Gutierrez, J. Lan, R. Zenobi, P. Engel, E. Slack

Defining factors that influence chemical transformation rates in gut microbiota cultures grown ex vivo [AS-108]

Jacob Folz, ETH Zurich

R. Fernández, M. Stevanoska, G. Aichinger, S. J. Sturla*

Comprehensive Characterization of PLGA and Liposomal β -Carotene Nanocarriers in Simulated Gastrointestinal Fluids [AS-109]

Roman Fortunatus, Adolphe Merkle Institute, University of Fribourg

S. Balog, P. Taladriz-Blanco, B. Rothen-Rutishauser, A. Petri-Fink

Could mineralised textiles be considered as time capsules? [AS-110]

Clémence Iacconi, HEIA-FR, HES-SO

L. Hendriks, E. Desplanques, L. Robbiola, C. Portmann, N. Haghipour, L. Bertrand

Towards Streamlined Environmental Persistence Assays for Trace Organic Contaminants: Findings from High-Throughput Method Optimization and Biodegradation Testing [AS-111]

Chiel Kaal, Eawag, Dübendorf

S. Partanen, N. Müller, K. Fenner*

Cost-Effective Method for Trace Elements Analysis in Solids by LA-N₂-MICAP-MS [AS-112]

Dylan Käser, ETH Zurich

T. Van Acker, B. Hattendorf, D. Günther*

Quantification of substances in exhaled breath using secondary electrospray ionization beyond MS measurements. [AS-113]

Timon Käser, ETH Zurich

S. Giannoukos, R. Zenobi*

Tracking Coordination Environment and Reaction Intermediates in Homo- and Heterogenous Epoxidation Catalysts via Ti L_{2,3}-edge NEXAFS [AS-114]

Lukas Lätsch, ETH Zurich

S. A. Guda, V. Romankov, C. Wartmann, J. Dreiser, A. Berkessel,

A. A. Guda, C. Copéret*

Development of a Total N-Nitrosamines Analyzer and Its Optimization for Real Water Applications [AS-115]

Woongbae Lee, EPFL Lausanne

M. Lee, F. Breider, U. von Gunten*

A quantitative targeted GC-MS approach to characterize lactose malabsorption [AS-116]

Kashish Mallick, ETH Zurich

C. Blaser, G. Pimentel, A. Vadakkechira, R. Guillod, G. Vergères,

R. Zenobi, D. Pohl, S. Giannoukos, K. J. Burton-Pimentel

Nanoscope mechano-imaging in polymers [AS-117]

Hrishikesan Pattam, Adolphe Merkle Institute, University of Fribourg

J. Clough*

First insights in untangling bulk ¹⁴C dates in painted artwork through Compound Specific Radiocarbon Analysis [AS-118]

Lionel Rumpf, HEIA Fribourg

L. Hendriks*, S. Szidat*

Bee bread collected by honey bees (*Apis mellifera*) as a terrestrial pesticide biomarker to complement water studies [AS-119]

Samira Stalder, Agroscope

M. Fracheboud, A. Stalder, B. Droz, A. C. Chiaia-Hernandez*, C.

Kast*

High resolution Imaging of Dawsonite using LA-ICP-TOFMS [AS-120]

Barbara Umfahrer, ETH Zurich

P. S. Garofalo, D. Günther*

Discovering breath metabolic profiles associated with lactose metabolism using secondary electrospray ionization mass spectrometry [AS-121]

Albin Vadakkechira, ETH Zurich

K. Mallick, R. Guillod, G. Vergères, R. Zenobi, D. Pohl, K. J.

Burton-Pimentel, S. Giannoukos*

Tracking cyanobacterial toxins and their biotransformation in Swiss surface waters [AS-122]

Xuejian Wang, Eawag, Dübendorf

S. Wullschleger, E. M.-L. Janssen*

Computational Chemistry [CC] Poster Session

Heavy-atom tunnelling in singlet oxygen predicted with ab-initio instanton theory [CC-101]

Imaad Ansari, ETH Zurich

G. Trenins, J. O. Richardson, E. R. Heller*

Cooperative free energy: correlation, solvation, and conformation in protein-ligand-protein ternary complexation [CC-102]

Shu-Yu Chen, ETH Zurich

R. Solazzo, M. Fouche, H. Roth, B. Dittrich, S. Riniker*

Structure Determination of Single Crystal Quartz by Hirshfeld Atom Refinement [CC-103]

Kanghyun Chu, University of Bern

Y. Balmohammadi, S. Grabowsky*

Predicting Off-targets from ChEMBL Data Using the Polypharmacology Browser [CC-104]

Maedeh Darsaraee, University of Bern

J. Reymond, J. Reymond*

Studying ion and water flow through aerolysin nanopores using molecular dynamic simulations [CC-105]

Jingze Duan, University of Geneva

L. Perrin, C. Cao

Accurate tunnelling splittings with second-order instantons [CC-106]

Jindřich Dušek, ETH Zurich

J. E. Lawrence, J. O. Richardson*

Performance of the new non-decomposable approximant for the non-additive kinetic potential for embedded radical [CC-107]

Tanguy Englert, University of Geneva

T. A. Wesolowski*

Data augmentation leads to near quantitative single-step round-trip accuracy in transformer-based retrosynthesis models [CC-108]

Yves Grandjean, University of Bern

D. Kreutter, J. Reymond*

Structure-based machine learning models to predict environmental biodegradation half-lives and their uncertainty [CC-109]

Jasmin Hafner, University of Zurich/Eawag

J. Cordero, A. Scheidegger, K. Fenner*

Spin-flip TDDFT within the Sternheimer formalism [CC-110]

Luis Hernandez Segura, University of Zurich

S. Lubner*

Reaction prediction in the low-data regime with transition state descriptors [CC-111]

Lauriane Jacot-Descombes, ETH Zurich

J. Landis, K. Jorner*

Sampling strategies for expectation values within the Herman-Kluk approximation [CC-112]

Fabian Kröniger, EPFL Lausanne

C. Lasser*, J. Vaníček*

Multiscale simulations of hybrid halide-perovskite photovoltaic devices [CC-113]

Nikolaos Lempesis, EPFL Lausanne

V. Carnevali, L. Agosta, V. Sláma, A. Vezzosi, U. Röthlisberger*

MiMiC Framework for Multiscale Simulations: Current Status and Recent Advancements [CC-114]

Andrea Levy, EPFL Lausanne

A. Antalík, U. Röthlisberger*

Nonadiabatic dynamics simulations in periodic condensed phase systems and challenges with hybrid-based Δ SCF [CC-115]

Momir Mališ, University of Zurich

E. Vandaele, S. Lubner*

Abraham solvation parameters model in the frame of graph convolutional neutral networks [CC-116]

Miroslava Nedyalkova, Fribourg University

A. Paluch, M. Lattuada

Molecular dynamics simulation of aerolysin nanopore using high-resolution cryo-EM structure [CC-117]

Louis Perrin, University of Geneva

J. Anton, I. Iacovache, J. F. Bada Juarez, L. A. Abriata,

M. J. Marcaida Lopez, M. Dal Peraro, B. Zuber, C. Cao*

Reactivity prediction of highly flexible catalysts using conformationally enriched machine learning [CC-118]

Stefan Schmid, ETH Zurich

C. Ser, M. Skreta, A. Aspuru-Guzik*, K. Jorner*

Cost-Informed Bayesian Reaction Optimization [CC-119]

Alexandre Schoepfer, EPFL Lausanne

J. Weinreich, R. Laplaza, J. Waser*, C. Corminboeuf*

Assessing the performance and accuracy of Delta Self-Consistent Field (Δ SCF) method within Restricted-Open Kohn-Sham formalism [CC-120]

Andrey Sinyavskiy, University of Zurich

M. Mališ, S. Lubner*

Predicting Reaction Properties using SMILES/CGR [CC-121]

Giustino Sulpizio, ETH Zurich

K. Jorner*

Striking the right balance of encoding electron correlation in the Hamiltonian and wavefunction ansatz [CC-122]

Kalman Szenes, ETH Zurich

M. Reiher

Computational insights into organic halide perovskite solar devices [CC-123]

Andrea Vezzosi, EPFL Lausanne

N. Lempesis, V. Carnevali, V. Sláma, U. Röthlisberger*

Ligand-based 3D Pharmacophore Search for Drug Analogues in Ultra-Large Combinatorial Libraries [CC-124]

Modest von Korff, Alipheron AG

T. Sander

3-Dimensional descriptors of molecular lipophilicity of macrocycles [CC-125]

Franz Waibl, ETH Zurich

F. Dey, S. Riniker*

Stochastic Sampling around Ring-Polymer Instanton [CC-126]

Yu-Chen Wang, ETH Zurich

J. Richardson

Microkinetic Molecular Volcano Plots for Enhanced Catalyst Selectivity and Activity Predictions [CC-127]

Thanapat Worakul, EPFL Lausanne

R. Laplaza, S. Das, M. Wodrich, C. Corminboeuf*

**Catalysis Sciences & Engineering [CE]
Poster Session**
Controlled Sulfur-Doping of Transition Metal Phosphides Enhances their Catalytic Properties [CE-101]

Nina Arnosti, University of Basel
V. Wyss, M. F. Delley*

Insight into structure-activity relationships of SiO₂-supported bimetallic Pd-Fe catalysts for CO₂ hydrogenation to methanol [CE-103]

Angelo Bellia, ETH Zurich
P. M. Abdala, C. R. Müller*

Air Compatible Alkali Metal Amide Catalysed Hydroamination of Heterocumulenes [CE-104]

Sophia Belrhomari, University of Bern
E. Hevia*

Mechanochemically derived iron atoms on defective boron nitride for stable propylene production [CE-105]

Gian Marco Beshara, ETH Zurich
I. Surin, M. Agrachev, H. Eliasson, T. Otroshchenko, F. Krumeich, G. Jeschke, R. Erni, E. V. Kondratenko, J. Pérez Ramírez*

Hydrogenation of CO₂ over Carbon-Supported NiGa and PdGa Catalysts: Influence of Ga-Precursor Choice on Catalytic Performance [CE-107]

Enzo Brack, ETH Zurich
M. Plodinec, C. Copéret*

The new Debye beamline at SLS2.0: a versatile platform for operando X-ray chemical and structural analysis with multimodal X-ray absorption spectroscopy and scattering [CE-108]

Adam Clark, Paul Scherrer Institute PSI, Villigen
S. Hitz, M. Nachttegaal

A scalable dynamic flow reactor for challenging continuous processes [CE-109]

Kim-Long Diep, HEIA Fribourg
E. Buchs, M. Moser, F. Steinemann, A. Georg, M. Dabros, R. Marti*

Electrochemical nitrate to ammonia reduction with a dendritic MoO_x catalyst [CE-110]

Robin Dürr, ETH Zurich
Y. Xu, D. F. Abbott, T. N. Huan, V. Mougel*

Shedding Light on the Synergistic Effects in Multi-Metal Solid Catalysts by Advanced Operando Spectroscopy [CE-112]

Nina Genz, Paul Scherrer Institute PSI, Villigen
F. Meirer, B. Weckhuysen

Convergent active site evolution of platinum single-atom catalysts for acetylene hydrochlorination and implication for toxicity minimization [CE-113]

Vera Giulimondi, ETH Zurich
M. Vanni, S. Damir, T. Zou, S. Mitchell, F. Krumeich, A. Ruiz-Ferrando, N. López, J. Gata-Cuesta, G. Guillén-Gosálbez, J. Smit, P. Johnston, J. Pérez-Ramírez*

Doped NiO yields ultra-low overpotential electrocatalysts in alkaline media – towards practical anion exchange membrane electrolyzers [CE-114]

Aswin Gopakumar, Institut Català d'Investigació Química (ICIQ)
J. Lloret-Fillol*

Precursors of Ethylene Oxide and CO₂ in Ethylene Epoxidation: In-Situ AP-XPS Study Revealing Absence of OMC Species on Ag foil [CE-115]

Man Guo, Paul Scherrer Institute PSI/ETH Zurich
N. Dongfang, M. Iannuzzi, J. A. Bokhoven, L. Artiglia*

Graphitic carbon nitride (g-C₃N₄) modified by ionic liquids for an improved water-splitting performance [CE-116]

Stefanie Kammereck, University of Zurich
G. R. Patzke*

Formation and Stability of μ₂-Peroxo on Titanosilicates, Anatase, and Rutile: Implications for Zeotype Catalysts [CE-117]

Christoph Kaul, ETH Zurich
L. Lätsch, I. Müller, T. De Baerdemaeker, A. Parvulescu, K. Seidel, H. Teles, N. Trukhan, C. Copéret*

Glycosyl Benzoates as Novel Donors for Glycosynthases [CE-118]

David Lim, University of Bern
S. de Lorenzo, L. Pillet, F. Paradisi*

Metal-Organic Framework-based catalysts for CO₂-to-methanol process [CE-119]

Anna Liutkova, Paul Scherrer Institute
F. A. Peixoto Esteves, E. Poghosyan, M. Ranocchiaro*

Enhancing catalyst effectiveness in chemical polyolefin recycling [CE-120]

Antonio Martín, ETH Zurich
S. D. Jaydev, D. García, K. Chikri, J. Pérez-Ramírez*

Ligand-replaced asymmetric inorganic-organic hybrids for highly active biomass assisted electrocatalytic water splitting [CE-121]

Lingshen Meng, University of Zurich
G. Patzke

Structure - catalytic performance relationship of modified SAPO-34 for methanol-to-olefins (MTO) reaction [CE-122]

Monika Mielniczuk, Paul Scherrer Institute / ETH Zurich
F. J. Dubray, J. A. van Bokhoven*

Flexibilisation of methanol synthesis from CO₂ by alternating carbon capture and utilization [CE-123]

Emanuele Moiola, Paul Scherrer Institute PSI, Villigen
A. Pappagallo, H. Petremand

The path to a versatile and biocompatible organometallic NAD(P)H regeneration system using an ¹⁸PYE⁺ complex [CE-124]

Laura Monte, University of Bern
N. Lentz, F. Paradisi*, M. Albrecht*

Optimizing Enzymatic Cascades for Halogenated L-Pipecolic Acid Production [CE-125]

Arpita Mrigwani, University of Bern
F. Paradisi*

High-Loading Pd-Phthalocyanine Covalent Organic Framework based SACs for Cross-Coupling Reactions [CE-126]

Murad Najafov, University of Fribourg
K. Song, S. Pollitt, F. Gándara, M. Nachttegaal *, A. Coskun*

Highly Efficient Homogeneous Catalyst For N₂O Hydrogenation and the Key Role of Water: Proton shuttling and H₃O₂- structures [CE-127]

Sven Nappen, ETH Zurich
A. Thomas*, H. Grützmacher*, M. Trincado

Ti-doping in silica-supported Ru methanation catalysts [CE-128]

Aurélien Neraud, ETH Zurich
W. Zhou, C. Copéret*

SiO₂-Supported CoPt_{1-x} Nanoalloys for the Dry Reforming of Methane [CE-129]

David Niedbalka, ETH Zurich
L. Thommen, P. M. Abdala, C. R. Müller*

Controllable production of single-walled and multi-walled carbon nanotubes in CH₄ catalytic pyrolysis using Fe-Mo/MgO [CE-130]

Zeyou Pan, Paul Scherrer Institute PSI, Villigen
J. van Bokhoven*

Unraveling the Promoting Effect of Diamine-Modified Metal-Organic Frameworks on the Ruthenium-Catalyzed CO₂ Hydrogenation to Methanol [CE-131]

Fabio Peixoto Esteves, ETH Zurich/ PSI
J. A. van Bokhoven, M. Ranocchiaro*

Insights into reduction of activated double bonds in flow using ene-reductases [CE-132]

Lauriane Pillet, University of Bern
M. R. Busch, D. Roura Padrosa, C. Fernández Regueiro, F. Paradisi*

Phosphine activity descriptors for palladium single-atom heterogeneous catalysts in cross-couplings [CE-133]

Dario Poier, HEIA Fribourg / ETH Zurich
O. Loveday, E. Lucas, M. Usteri, D. Stoian, G. Guillén-Gosálbez, N. López, S. Mitchell, R. Marti*, J. Pérez-Ramírez*

Manganese complexes bearing bidentate PYE ligands for formic acid dehydrogenation [CE-134]

Sabela Reuge, University Bern
N. A. Lentz, M. Albrecht*

Defects in Metal Oxides and their Effects on Catalysis [CE-135]

Anies Rösch, University of Basel
V. Wyss, M. F. Delley*

Data-driven tools for enzyme immobilization - auxiliary enzymes are case study [CE-136]

David Roura Padrosa, inSEIT AG
C. L. Fernández Regueiro, V. Marchini

Promotional Effects of Si Addition to Alumina-based Pt-Ga Systems on Catalyst Stability for Propane Dehydrogenation Reaction [CE-137]

Kazutaka Sakamoto, ETH Zurich
M. Plodinec, E. Lam, C. Copéret*

Directed Evolution and Modification of an Artificial Hydroxylase Based on a Thermostable Human Carbonic Anhydrase [CE-138]

Elias Salvisberg, University of Basel
I. Morita, K. Zhang, A. Faraone, R. P. Jakob, T. Maier, A. Vorobieva, B. Correia, T. R. Ward*

Organic Groups on a Transition Metal Phosphide Catalyst Tune Hydrogenation Reactions [CE-139]

Yu-Chun Shen, University of Basel
M. F. Delley*

Atomically dispersed palladium-platinum catalysts from defined precursors [CE-140]

Rosie Somerville, EPFL Lausanne
J. Schmidt, E. Lam, D. Stoian, P. J. Dyson*

High-Pressure Grazing Incidence Cell for *In Situ* XAS Characterization of Nanoparticles on Planar Substrates under CO₂ Hydrogenation Conditions [CE-141]

Sumant SumantPhadke, Paul Scherrer Institute PSI, Villigen
J. Coroa, I. Abbas, J. Yin, D. Grandjean, E. Janssens, O. V. Safonova*

The role of metal nanostructure in ceria-supported catalysts for ammonia oxidation to nitrous oxid [CE-142]

Ivan Surin, ETH Zurich
Q. Yang, F. Krumeich, T. Otroshchenko, V. A. Kondratenko, E. V. Kondratenko, J. Pérez-Ramírez*

Ru-NHC Complexes for the Hydroesterification of Alkenes [CE-144]

Roland Turnell-Ritson, EPFL Lausanne
R. Descroches, P. J. Dyson*

Understanding and controlling activity and selectivity patterns of Pd₁@C₃N₄-catalyzed Suzuki-Miyaura couplings [CE-145]

Marc-Eduard Usteri, ETH Zurich
G. Giannakakis, A. Bugaev, J. Pérez-Ramírez, S. Mitchell, J. Pérez-Ramírez*, S. Mitchell*

Epoxidation of Olefins by Cobalt Sulfide and its Parallels to Oxygen Evolution Reaction Electrocatalysis [CE-146]

Vanessa Wyss, University of Basel
I. A. Dinu, L. Marot, C. G. Palivan, M. F. Delley*

Directed dual charge pumping tunes the d-orbital configuration of Pt cluster boosting hydrogen evolution kinetic [CE-147]

Zeyi Zhang, University of Zurich

Design of technical ZnO/ZrO₂ catalysts for green methanol synthesis [CE-148]

Tangsheng Zou, ETH Zurich
T. P. Araújo, M. Agrachev, X. Jin, F. Krumeich, G. Jeschke, S. Mitchell, J. Pérez-Ramírez*

Are Pt-based catalysts always necessary for hydrogen and oxygen recombination reactions? [CE-149]

Zohreh Akbari, EPFL Valais
A. Züttel*

Elucidating the mechanism of Fe incorporation in in situ synthesized Co-Fe oxygen-evolving nanocatalysts [CE-150]

Thi Ha My Pham, EPFL Valais
T. Shen, V. Tileli*

Chemistry and the Environment [EV] Poster Session**Bridging the Gap Between Laboratory and Environmental Photochemistry [EV-101]**

Sofia Ambrogetti, ETH Zurich
J. Laszakovits, S. Partanen, K. McNeill*

Ozonation of 4 pesticides: substitution effect on ozone reactivity and adsorbability of transformation products on granular activated carbon [EV-102]

Lucie Bertolaso, EPFL Lausanne
C. Gachet Aquillon, M. Chipps, N. Revens, B. Jefferson, P. Jarvis, P. Campo, I. Carra, U. von Gunten*

Insights into Rhine Industrial Contamination: A Data Mining Approach to High-Frequency Measurements [EV-103]

Teofana Chonova, Eawag, Dübendorf
S. Ruppe, I. Langlois, D. Griesshaber, M. Loos, M. Honti, K. Fenner*, H. Singer*

EQS Derivation of a Widely Used Type I Pyrethroid: Tefluthrin [EV-104]

Breanne Holmes, Eawag, Dübendorf
M. Junghans

Legacy and current pesticide residues from agricultural soil and drainage water challenge risk assessment models [EV-105]

Karel Hornak, Agroscope
S. Mangold, N. Bartolomé, I. Hilber, T. Bucheli*

Determining the proteolytic fingerprint of Lake Geneva to investigate the mechanism of virus inactivation in lake water [EV-108]

Josephine Meibom, EPFL Lausanne
N. Wichmann, M. Zumstein, T. Kohn*

Urban Halocarbon Measurements in Switzerland [EV-109]

Michelle Müller, Empa
M. K. Vollmer, P. Schlauri, P. Rubli, L. Emmenegger, S. Reimann*

Insights into reaction mechanisms for the ozonation of primary amines applying nitrate formation kinetics, $\delta^{15}\text{N-NO}_3^-$ and ^{18}O -labeling [EV-110]

Jiwoon Ra, Eawag, Dübendorf
U. von Gunten*

Reactions of N,O- and N,S-azoles with ozone: kinetics and mechanisms [EV-111]

Simon Rath, Eawag / EPFL
U. von Gunten*

New versus Naturally Aged Greenhouse Cover Films: Degradation and Micro-Nanoplastics Characterization under Sunlight Exposure [EV-112]

Patricia Taladriz-Blanco, Adolphe Merkle Institute
C. Sorasan, L. Rodriguez-Lorenzo, B. Espiña, R. Rosal, P. Taladriz-Blanco*

Leveraging modern assessment methods to shed light on the environmental impact of a century of military activities in Switzerland [EV-113]

Chloé Udressy, Eawag, Dübendorf
J. Hollender, R. Kägi, A. Gassner, T. B. Hofstetter*

Participation in the intergovernmental science-policy panel on chemicals, waste and pollution prevention [EV-114]

Zhanyun Wang, Empa

**Inorganic Chemistry [IC]
Poster Session****Simple Yet Complex: Azides and Azidometallates [IC-101]**

Semih Afyon, Belenos Clean Power Holding Ltd.

Neopentyl Sodium as a Tool for Metalation of Non-Activated Alkenes [IC-102]

David Anderson, University of Bern
E. Hevia*

Towards the Elucidation of Ni-Catalyzed Cyclopropanation: MeNiGaL – a Ni(0) Methyl Complex Based on a Ni-Ga Double-Decker Complex [IC-103]

Maurice Andrey, ETH Zurich
A. Bütikofer, R. Wolf, S. A. Künzi, P. Chen*

Functionalized Terthiophenes as Multi-Electron Electrolytes for Energy Storage [IC-104]

Máté Bezdek, ETH Zurich
D. Käch

Toward predicting silver ion binding in proteins [IC-105]

Alexandre Bianchi, University of Fribourg
F. Marquet, L. Manciocchi, M. Spichty, K. M. Fromm*

Synthesis and Reactivity of Triazolylidene-Group 10 Metal Complexes via Oxidative Addition of 5-Halo-Triazolium Salts [IC-106]

Fabienne Bühler, University of Bern
G. Rigoni, M. Albrecht*

Cyclopentadienone Monoisocyanide Iron Complexes: Synthesis and Catalytic Performance in Transfer Hydrogenation [IC-107]

André Bütikofer, ETH Zurich
D. Svoboda, P. Chen*

Towards Understanding Electrochemical Interfaces: An interplay of chemical interactions and electric fields [IC-108]

Tzu-Chin Chang Chien, University of Basel
M. F. Delley*

A palladium-based coordination cage for selective lithium binding [IC-109]

Damien Chen, EPFL Lausanne
K. Severin*

Aluminum Transfer at Zinc and Copper [IC-110]

Fabian Dankert, University of Bern
E. Hevia*

Palladium-based cages of low symmetry [IC-111]

Jean de Montmollin, EPFL Lausanne
R.-J. Li, A. B. Solea, D. W. Chen, P. Gorrea Acín, F. Fadaei-Tirani, R. Scopelliti, K. Severin*

N-heterocyclic carbene tailoring allows tuning of iron-catalysed C–H amination [IC-112]

Luke Hudson, University of Bern
M. Albrecht*

Uncovering the Super Basic and Nucleophilic Reactivities of Co(II) Amide $\text{Co}(\text{TMP})_2$ [IC-113]

Na Jin, University of Bern
A. Logallo, E. Hevia*

Structure and reactivity of a rhenium(VII)-methylidyne complex [IC-114]

Péter Pál Kalapos, ETH Zurich
P. Chen*

Metal template synthesis of aromatic tridentate ligand for studying the stability of lanthanide complexes in solution and solid state [IC-115]

Giau Le-Hoang, University of Geneva
L. Guenée, Q. Sommer, C. Piguet*

Bio-Inspired Molecular Oxygen Evolution Catalysts with $\{\text{Co}_4\text{O}_4\}$ Cubanes Embedded in a Conducting Polymer [IC-116]

Shangkun Li, University of Zurich
Z. Zhang, W. Marks, X. Huang, H. Chen, D. Stoian, R. Erni, C. Triana, G. Patzke*

Design and characterization of new sensors based on functionalized organometallic cages for the selective detection of sugars and other analytes [IC-117]

Alaa Maatouk, University of Neuchatel
T. Rossel, B. Therrien*

Mechanistic Investigations of Metal-Oxo Cubane Formation [IC-118]

Walker Marks, University of Zurich
K. F. Würzer, G. R. Patzke*

Chemical and Redox Non-Innocence in Low Valent Molybdenum β Diketonate Complexes: Novel Pathways for CO₂ and CS₂ Activation [IC-119]

Fabio Masero, ETH Zurich
V. Mougel*

Revisiting Early-Stage Coordination Chemistry: Exploring the Phosphorus Analogue of Hydroxylamine [IC-120]

Sven Nappen, ETH Zurich
H. Grützmacher*

Exploring New Methathesis Routes to Access Calcium Organometallics [IC-121]

Andrew Platten, University of Bern
E. Hevia*

Probing of BDFEs of surface Pd-H across solvent environments and applications thereof [IC-122]

Lok-Nga Poon, ETH Zurich
V. Mougel*

Salen-derived heterometallic complexes [IC-123]

Jocelyn Pradegan, University of Fribourg
A. Crochet, K. M. Fromm*

Synthesis and Understanding of Donor Flexible Thioamide Ligands [IC-124]

Taj Seaton, University of Bern
M. Albrecht*

Hetero- and homometallic complexes based on (iso)-nicotinic acid [IC-125]

Claudia Tringali, University of Fribourg
K. M. Fromm*

New Frontiers in Organocaesium Chemistry: Advances with Caesium Amides [IC-126]

Alex Truong, University Bern
D. E. Anderson, E. Hevia*

Atomically precise surface chemistry of zirconium and hafnium metal oxo clusters beyond carboxylate ligands [IC-127]

Ajmal Roshan Unniram Parambil, University of Basel
R. Pokratath, M. Parammal, D. Van den Eynden, E. Dhaene, A. Prescimone, P. Shahgaldian*, J. De Roo*

Speciation and Profiling of Bulky Chiral Cyclopentadienyl Cobalt Complexes [IC-128]

Bram Van Den Bossche, EPFL Lausanne
N. Cramer*

Synthesis and Catalytic Applications of Highly Reduced Heterobimetallic Nickelates [IC-129]

Luca Vedani, University of Bern
A. M. Borys, E. Hevia*

Controlled Heteroelement-Transfer onto Transition Metal Phosphide Surfaces [IC-130]

Gregor Wasser, University Basel
M. F. Delley*

The coordination chemistry of di(2-pyridyl) ketone: Structural versatility and synthetic strategies of the Co²⁺/Zn²⁺ chemistry with the ligand di(2-pyridyl) ketone [IC-131]

Katrin Würzer, University of Zurich
W. R. Marks, G. R. Patzke*

Reactivity of Diazoolefins [IC-132]

Bastiaan Kooij, EPFL Lausanne
K. Severin*

**Medicinal Chemistry & Chemical Biology [MC]
Poster Session**

Stereochemistry of Cell Penetrating Peptides [MC-101]

Yasien Amer, University of Bern
J. Reymond*

Synthesis of GBD Derived Bicyclic Diamine as Interesting Scaffold for Medicinal Chemistry [MC-102]

Giulia Baldoni, University of Bern
J. Reymond*

Natural product drug discovery pipeline reveals ellagic acid to reduce forgetting in *Caenorhabditis elegans* through specific Musashi inhibition [MC-103]

Tamara Balsiger, University of Basel
R. Hagmann, K. Huynh, P. Solis, M. Hamburger, A. Papassotiropoulos, R. Teufel, A. Stetak*, E. Garo*

A versatile "Synthesis Tag" (SynTag) for the chemical synthesis of aggregating peptides and proteins [MC-104]

Héloïse Bürgisser, University of Zurich
E. Williams, R. Lescure, A. Premanand, A. Jeandin, N. Hartrampf*

Synthesis and activity of novel acylfulvene analogs appended with covalent reactive groups [MC-105]

Dan Dempe, ETH Zurich
L. Slappendel, O. Schärer, S. Sturla*

3D dynamic hydrogel matrix for cultivation of intestinal organoids [MC-106]

Yves Erdin, University of Basel
P. Fluechter, C. Schneider, M. Nash, Z. Korb*

Catalytic improvement of a metalloenzyme using hydrophobic tuning with non-canonical amino acids [MC-108]

Sandro Fischer, University of Zurich
A. Natter Perdiguero, A. Deliz Liang*

Development of novel bitopic and bifunctional ligands to study adenosine A1 receptors [MC-109]

Maren Flaßhoff, University of Bern
T. Sarvanathan, A. Pearce, G. Ladds, M. Lochner*

Development and physicochemical characterization of novel anthranilic anilide-based TRPM4 channel inhibitors identified by extensive SAR-study [MC-110]

Christian Gerber, University of Bern
D. Ross-Kaschitza, B. Augustynek, P. Grossenbacher, S. A. Singer, C. Peinelt, M. Lochner*

Discovery of indolicidin diastereomers as antimicrobial agents [MC-111]

Xiaoling Hu, University of Bern
M. Orsi, J. L. Reymond*

A Deep Learning Model for Predicting the Thermal Stability of Collagen Triple Helices [MC-112]

Kiseop Im, ETH Zurich
I. Warm, H. Wennemers*, T. Fiala*

Chemical Probe to Visualize Bacterial Physiology: A ratio-metric pH Sensor for Gram-positive and Gram-negative Bacteria [MC-113]

Dorothea Kossmann, University of Zurich
A. Iizuka, N. Khanna*, P. Rivera-Fuentes*

A HaloTag-based Gene Expression Reporter System for Live-Cell Imaging [MC-114]

Henriette Lämmermann, University of Zurich
J. Nguyen, J. Tamez Fernández, F. Kuttler, J. Bortoli Chapalay,
M. Chambon, G. Turcatti, P. Rivera Fuentes*

Engineering a Zinc-Dependent Phosphotriesterase with a Non-Canonical Histidine Derivative [MC-115]

Benjamin Manser, University of Zurich
A. Deliz Liang*

Ligand-directed bioconjugation on native protein with hypervalent iodine-based Ethynylbenziodoxolones (EBXs) reagents [MC-116]

Christine Marty, EPFL Lausanne
X. Ji, C. Heinis*, J. Waser*

Synthesis of modified carbohydrates as glyco-donors aiming complex glycans synthesis and glycopeptides [MC-117]

Matheus Meirelles, University of Bern
K. P. Locher*, J. Reymond*

Protein Engineering with Genetic Code Expansion [MC-118]

Anton Natter Perdiguero, University of Zurich
P. A. Lugon, A. D. Liang*

Examining the interaction between thiolate protected metal clusters and lipid bilayers [MC-119]

Merve Örer, University of Geneva
T. Bürgi*

Similar Structure, Different Effects: Investigation of Pt(II) Complexes as DNA-Targeting Antibiotics against Gram-positive Bacteria [MC-120]

Cagri Özsan, University of Bern
A. Schäfer, M. L. Fulgencio, A. Frei *, M. Wenzel*

Evaluating Lysyl Oxidase Activity with Turn-On Fluorescent Probes [MC-121]

Laura Poller, ETH Zurich
H. Wennemers*

Nano-carrier Encapsulated Chlorin e6 and its Derivatives as Photosensitizers for Dermal Application: Investigating their Incorporation into Lipid Carriers and Skin Penetration [MC-122]

Jirachaya Pongnoppa, University of Bern
J. Furrer, S. Kaessmeyer, H. Roess, G. Vorburger Schmidt, M. Vermathen*

Synthesis of novel bicyclic diamine scaffolds derived from tropinone. [MC-123]

Austia Puckett, University of Bern
J.-L. Reymond*

Single-Molecule Peptide and Protein Identification using Fluorescence Blinking Fingerprints [MC-124]

Salome Püntener, University of Zurich
K. Bielec, P. Rivera-Fuentes*

Synthesis of Chiral Tricyclic Piperazine Scaffolds from the GDB Database [MC-125]

Leon Rebhan, University of Bern; J.-L. Reymond*

Peptide-stabilized gold nanoparticles [MC-126]

Alžbeta Runová, ETH Zurich
H. Wennemers*

Beyond static structures: The dynamic impact of Introna B on fungal ribozymes [MC-127]

Abdul Rahman Sadiq, University of Zurich
S. Zelger-Paulus*, R. K.O. Sigel*

Amphipathic proline-rich cell penetrating peptides for mitochondria targeting [MC-129]

Adeline Schmitt, ETH Zurich
H. Wennemers*

Click-chemistry-enabled elucidation of transcriptional effects of DNA oxidation at a genome-wide level [MC-130]

Navnit Singh, ETH Zurich
V. Takhaveev, M. Rulka, N. Püllen, S. J. Sturla*

Development of lysine-targeting DNA Probes to disrupt XPG-mediated Nucleotide Excision Repair for cancer therapy. [MC-131]

Laura Slappendel, ETH Zurich
D. P. Dempe, J. Huber, O. Schärer, S. J. Sturla*

Assessing gut microbiota's role in phytoestrogen bio-activation [MC-132]

Maja Stevanoska, ETH Zurich
K. Beekmann, S. Sturla*, G. Aichinger*

Potent Inducers of Paraptosis Through Electronic Tuning of Michael Acceptors [MC-133]

Juan Tamez-Fernández, University of Zurich
J. Nguyen, P. Rivera-Fuentes*

Non-invasive in vivo Determination of Potassium in Human Muscle by 39K MR Spectroscopy on a 7T MR Scanner. A Feasibility Exercise Study. [MC-134]

Marc Thiede, University of Bern
E. Rösli, H. H. Primasová, B. Vogt, P. Vermathen*

Probing the Penetration of Encapsulated Photosensitizers into Skin Models [MC-135]

Tyrone Wyss, University of Bern
S. Kaessmeyer*, H. Roess, G. Vorburger, I. Gjuroski, J. Furrer, M. Vermathen*

Photosensitizers in Targeted Photodynamic Therapy of Colorectal Cancer [MC-136]

Yueying YANG, University of Neuchatel and cnam
M. Saho, N. Lagarde, B. Therrien*, M. Sylla*

A Drug-like Library of Structurally Diverse Spirocyclic Saturated N-Heterocycles [MC-137]

Elia Boschi, ETH Zurich
D. Mazunin, D. Wechsler, A. Topp, T. Killian, A. Müller, C. Kroll, W. Haap*, J. Bode1*

**Organic Chemistry [OC]
Poster Session****Enantioselective Total Synthesis of (+)-Aberrarone [OC-101]**

Willi Amberg, ETH Zurich
E. M. Carreira*

Fluorescent Membrane Probes for Increased Partitioning in Membranes [OC-102]

Felix Bayard, University of Geneva
X. Chen, N. Sakai, S. Matile*

Selective Recognition of Sucrose in Water by a Synthetic Receptor [OC-103]

Lena Beiersdörfer, ETH Zurich
M. Li, D. Zetschok, H. Wennemers*

Oxidative amination of unactivated alkenes via nitrogen atom insertion into carbon-carbon double bonds [OC-104]

Yannick Brägger, ETH Zurich
B. Morandi*, A. K. Paschke, N. Nasiri, B. B. Botlik, F. Felician

Catalytic Difunctionalization of Cyclopropenes via a Tethering Strategy [OC-105]

Duncan Brownsey, EPFL Lausanne
A. Schöpfer, J. Waser*

Catalyst Control Over Pentavalent Stereocenters [OC-106]

Anton Budeev, University of Basel
J. Dong, D. Häussinger, C. Sparr*

Reversing the Diastereoselectivity of the Organocatalyzed Conjugate Addition Reactions to Nitroolefins – From Reaction Development to Formal Synthesis of Upadacitinib [OC-107]

Alena Budinska, ETH Zurich
A. Berg, M. Heinke, H. Wennemers*

Organic Dye Photocatalyzed Synthesis of Functionalized Lactones and Lactams via a Cyclization-Alkynylation Cascade [OC-108]

Diana Cavalli, EPFL Lausanne
J. Waser*

Length-Dependant Uptake and Inhibition of Cell-Penetrating Poly(disulfide)s [OC-109]

Michaël Cognet, University of Geneva
F. Coelho, N. Sakai, S. Matile*

Iridium-Catalyzed Hydrogenation of Pyridines [OC-111]

Arthur Despois, EPFL Lausanne
N. Cramer*

Paracyclophenylenes as functional units and building blocks for SWCNTs [OC-112]

Jia Ding, University of Basel
M. Mayor*

Traceless photoremovable self-immolative amino acid linker [OC-113]

Maël Djaïd, University of Fribourg
C. Bochet*

Nitration Processes Using Bench-Stable Nitrating Reagents [OC-114]

Anthony Fernandes, University of Bern
V. Valsamidou, D. Katayev*

Bambusurils: Kinetically-Controlled Synthesis of Functionalized Anion-Binding Macrocycles [OC-115]

Tomas Fiala, ETH Zurich
J. Frei, T. Herentin, W. Nijskens, V. Sindelar

Fe(II)-catalyzed α C–H amidation of N-heterocycles [OC-116]

Andrea Geraci, University of Basel
O. Baudoin*

Solvent-Controlled Switchable Divergent Synthesis [OC-117]

Rahul Giri, University Of Bern
D. Katayev*

Eco-friendly anaerobic oxidation of aryl diazoesters with heterocyclic N-oxide under ball milling: Synthesis of 1,2-dicarbonyl systems [OC-118]

Souvik Guha, HEIA Fribourg
L. Gremaud*

Electric-Field Induced Asymmetric Enamine Catalysis [OC-119]

Shenyi Guo, University of Geneva
A. Jozeliunaite, M. Gallardo Villagran, M. Gutiérrez López, N. Sakai, S. Matile*

Enantioselective access to planar-chiral macrocyclophanes via Pd-catalyzed C–H arylation [OC-120]

Soohee Huh, University of Basel
E. Linne, O. Baudoin*

Aromatic Ring-Opening Metathesis [OC-121]

Valeriia Hutskalova, University of Basel
C. Sparr*

Towards shape-assisted self assemblies in solution [OC-122]

Nils Jansen, University of Geneva
M. Rickhaus*

Mechanistic studies on photochemical reactions: Is the Hammond postulate valid for *meta* effect induced photo-solvolysis of benzylic esters? [OC-123]

Gaël Jarjoura, University of Fribourg
C. G. Bochet*

Bifunctional Group Transfer [OC-124]

Mathias Kissling, University of Bern
R. Giri, E. Zhilin, S. Patra, A. J. Fernandes, D. Katayev*

Sodium-mediated Nucleophilic Amination of Pyridines [OC-125]

Jasmin Kocher, University of Bern
A. Tortajada, E. Hevia*

Pd-Catalyzed Dynamic Kinetic Resolution of Pillar[5]arenes [OC-126]

Antoine Konter, University of Geneva
C. Mazet*

Sustainable Beckmann Rearrangement using Bead-Milling Technology: The Route to Paracetamol [OC-128]

Rémy Mariaux, HEIA Fribourg
R. Geib, E. Colacino, L. Gremaud*

Chemical Surface Modifications [OC-129]

Jesús Mirón García, University of Basel
M. Mayor*

Mechanochemistry Drives Alkene Difunctionalization via Radical Ligand Transfer and Electron Catalysis [OC-130]

Subrata Patra, University of Bern
D. Katayev*

Ficini Reaction with Acrylates for the Stereoselective Synthesis of Aminocyclobutanes [OC-131]

Emma Robert, EPFL Lausanne; J. Waser*

Further Investigations on Excited State Potential Energy Surfaces: Can the Hammond Postulate be Applied to Photochemical Reactions? [OC-132]

Nicolas Rosa De Sousa, University of Fribourg
C. G. Bochet*

Investigating the Formation of Iodonitrene from Hypervalent Iodine Oxidants and Ammonia [OC-133]

Florian Ruepp, ETH Zurich
B. Morandi*

Axially-Chiral Boramidines for Detailed (Chir)Optical Studies [OC-134]

Nidal Saleh, University of Geneva
J. Lacour*

Chemoselective Approaches for the Discovery of Natural Products [OC-135]

Simon Sieber, University of Zurich

Photocatalytic Generation of Cyclopropenium Cations**[OC-136]**Vladyslav Smyrnov, EPFL Lausanne
J. Waser***Enamine Synthesis *via* Regiocontrolled 6-*endo-dig* and 5-*exo-dig* Tethered Carboamination of Propargylic Alcohols****[OC-137]**Helena Solé-Àvila, EPFL Lausanne
M. Puriñš, L. Eichenberger, J. Waser***Sodium catalysed borylation of arenes with Iminoboranes****[OC-138]**Clarence Tan, University of Bern
A. Tortajada, E. Hevia***Tailoring sodium organometallic reagents for catalytic deuteration and isomerization reactions****[OC-139]**

Andreu Tortajada, University of Bern; E. Hevia*

Photoswitching neutral homoaromatic hydrocarbons**[OC-140]**Trung Tran Ngoc, University of Zurich
N. Grabicki, E. Irran, O. Dumele, J. F. Teichert***1,4-Pd Shift-Enabled Synthesis of Fused 4-Membered Rings****[OC-141]**Maria Tsitopoulou, University of Basel
A. Clemenceau, P. Thesmar, O. Baudoin***Mechanochemical Nitration of Arenes and Alcohols Using Bench-Stable Organic Nitrating Reagent****[OC-142]**

Vasiliki Valsamidou, University of Bern

D. Katayev*

Under Control: π -Radical Cascades of Triangulene**[OC-143]**Paula Widmer, University of Zurich
L. Valenta, M. Mayländer, S. Richert, T. Šolomek*, M. Juríček***Towards the polymerization of Centrohexaindane****[OC-144]**Lara Wild, University of Geneva
K. Zhang, R. Jamagne, M. Rickhaus***Site-Selective Deuteration of (hetero)arenes Catalyzed by Supported Ir Nanoparticles****[OC-145]**

Chengbo Yao, ETH Zurich

C. Copéret*

Repurposing Myoglobin into an Abiological Asymmetric Ketoreductase**[OC-146]**

Xiang Zhang, NCCR Catalysis, Switzerland

D. Chen, J. Stropp, R. Tachibana, Z. Zou, D. Klose, T. R. Ward*

Synthesis and Self-Assembly of Contorted Aryl Amines**[OC-147]**

Kai Zhang, University of Geneva

N. Jansen, M. Rickhaus*

Access to Cyclic Borates by Cu-Catalyzed Borylation of Unactivated Vinylcyclopropanes**[OC-148]**

Cheng Zhang, University of Geneva

C. Mazet*

Pnictogen-Bonding Catalyzed Hydrogenation Reaction and Ion Transports in Vesicles**[OC-149]**

Qingxia Zhang, University of Geneva

G. Renno, N. Sakai, S. Matile*

Unlocking Molecular Design via Dihalogenation of Unsaturated Hydrocarbons**[OC-150]**

Egor Zhilin, University of Bern

R. Giri, D. Katayev*

An Evolved Artificial Radical Cyclase Enables the Construction of Bicyclic Terpenoid Scaffolds via an H-Atom Transfer Pathway**[OC-151]**

Dongping Chen, University of Basel

X. Zhang, A. A. Vorobieva, R. Tachibana, A. Stein, R. P. Jakob,

Z. Zou, D. A. Graf, A. Li, T. Maier, B. E. Correia*, T. R. Ward*

Physical Chemistry [PC]**Poster Session****Surface Immobilization of Magnetic Polymeric Giant Unilamellar Vesicles****[PC-101]**

S. narjes Abdollahi, University of Basel

D. Messmer, V. Mihali, C. Palivan*

Supramolecular Modulation for Hybrid Perovskite Photovoltaics**[PC-102]**

Ghewa AISabeh, EPFL/AMI

M. Graetzel*, J. V. Milic*, S. Kasemthaveechok, M. A. Ruiz-

Preciado, P. Zimmermann, D. Dekker, M. Galerne, E. Moulin,

F. T. Eickemeyer, S. Kasemthaveechok

Understanding the activation mechanism of Ru-based catalyst for CO₂ reduction via Ultrafast Transient-IR**[PC-103]**

Sergio Aranda Ruiz, University of Zurich

L. Tatarashvili, P. Hamm*

Polymer assembly as artificial cell for compartmentalizing lactate enzymatic reaction**[PC-104]**

Arianna Balestri, University of Basel

C. Palivan*

Charge-carrier dynamics in chiral gold nanoclusters**[PC-105]**

Tristan Blandenier, University of Basel

M. Oppermann*, T. Bürgi

Extending ultrafast spectroscopy to the deep ultraviolet with stretched hollow core fiber technology**[PC-106]**

Pieter Brongers, University of Basel

C. Brahms, M. Oppermann*

Use of NMR to study cubic phases for drug delivery in topical photodynamic therapy**[PC-107]**

Joel Bruegger, University of Bern

I. Gjuroski, P. Vermathen, J. Furrer, M. Vermathen*

Deciphering the oxygen evolution reaction mechanism on 3d transition metal oxides by using pump-probe X-ray absorption spectroscopy**[PC-108]**

Cheshta Chopra, Paul Scherrer Institute PSI, Villigen

E. Fabbri, M. Nachtegaal, T. J. Schmidt, G. Smolentsev*

Precision spectroscopy of Rydberg states in ⁴He and ³He**[PC-109]**

Gloria Clausen, ETH Zurich

F. Merkt*

pH-Responsive Nanocarriers Formed *via* an Improved Synthesis of PMOXa-*b*-PDPA Amphiphilic Block Copolymers**[PC-110]**

John Coats, University of Basel

A. Nikoletic, L. Heuberger, M. Korpidou, C. Schönenberger,

C. Palivan*

Second harmonic imaging of osmotic gradients**[PC-111]**

Nelson Correa Rojas, EPFL Lausanne

Z. Li, M. Eremchev, A. Roux*, S. Roke*

High-resolution liquid cell architecture for microsecond time-resolved cryo-EM [PC-112]

Wyatt Curtis, EPFL Lausanne

J. Hruby, S. V. Barrass, M. Drabbels*, U. J. Lorenz*

High-field optically induced NMR hyperpolarization in solids [PC-113]

Federico De Biasi, EPFL Lausanne

M. Visegrádi, M. Levien, G. Karthikeyan, M. A. Hope, Y. Qiu, P. J. Brown, M. R. Wasielewski, O. Ouari, L. Emsley*

Advancing polymer-based catalytic nanocompartments in localized drug production and delivery [PC-114]

Ionel Dinu, University of Basel

M. Korphidou, C. G. Palivan

Colloidal-ALD for hybrid QD@oxide core@shell structures to photocatalyze organic reactions [PC-115]

Marco Fabbiano, EPFL Lausanne

O. Segura Lecina, P. B. Green, R. Buonsanti*

Multiscale probing of interactions in aqueous ionic solutions [PC-116]

Mischa Flór, EPFL Lausanne

A. Bouchez, V. Vorobev, S. Roke*

The effect of pH on enzyme catalyzed lipolysis at the oil/water interface [PC-117]

Matteo Frigerio, University of Fribourg

S. Salentinig, M. Leser

Photoinduced Charge Transfer and Symmetry Breaking in Pyrrolopyrrole Based Quadrupolar Molecules [PC-118]

Chinju Govind, University of Geneva

E. Balanikas, R. F. Teran, G. Sanil, D. T. Gryko, E. Vauthey*

Using Gas-Phase FRET to Study the Structure of Diabetes-Related Polypeptides [PC-119]

Kim Greis, ETH Zurich

S. Huang, R. Wu, L. Benzenberg, R. Zenobi*

Gas-phase study of rotational-state and conformational effects in chemi-ionization reactions under single-collision conditions [PC-120]

Chao He, University of Basel; A. Mishra, L. Ploenes, P. Stranak, J. Kim, S. K. Kim, S. Willitsch*

Two-dimensional organic frameworks investigated by in-situ time-resolved spectroscopy [PC-121]

Isabelle Holzer, University of Bern

R. Guntermann, K. Muggli, T. Bein, N. Banerji*

The influence of the bipolaron formation rate on the charge transport properties of chemically doped oligoetherized polythiophene [PC-122]

Maximilian Horn, University of Bern

E. G. Röck, C. Kousseff, N. Banerji*, I. McCulloch*

Doping of Polythiophenes and Polythienothiophenes with Alkyl or Glycol Sidechains [PC-123]

Basil Hunger, University of Bern

D. Tsokkou, M. Horn, E. Röck, N. Banerji*

Structural Dynamics of SARS-CoV-2 Spike Proteins Revealed by Microsecond TimeResolved Cryo-EM [PC-124]

Subha Jana, EPFL Lausanne

M. Drabbels, U. J. Lorenz*

Precision Spectroscopy and Coherent Manipulation of a Single Molecular Nitrogen Ion [PC-125]

Richard Karl, University of Basel

A. Shlykov, M. Roguski, M. Diouf, S. Willitsch*

Detecting metal hyperfine couplings with chirped radio-frequency pulses in Electron Nuclear Double Resonance [PC-126]

Daniel Klose, ETH Zurich

J. Stropp, N. C. Nielsen, N. Wili

A soft X-ray absorption spectroscopy setup for liquid samples at SwissFEL [PC-127]

Jonas Knurr, EPFL Lausanne

K. Schnorr, A. Al Haddad, C. Bostedt*

Beyond Excited-State Symmetry Breaking in Donor–Acceptor–Donor Systems: Torsional Disorder, Redox Dependence and Synthetic Modifications [PC-128]

Joseph Kölbl, University of Geneva

R. J. Fernández-Terán*

Investigations on Fission Product Release Behavior for GEN-IV Nuclear Reactor Designs [PC-129]

Xuandong Kou, University of Bern

R. Eichler, E. Maugeri, R. Eichler*, E. Maugeri*

Synthesis and Properties of Ag₂₉ Nanocluster [PC-130]

Subhradip Kundu, University of Geneva

K. Ethmane, D. Canto, V. Muñoz, L. Llanes Montesino, A.

Rosspeintner, L. Lawson Daku, M. Pupier, J. Viger-Gravel*,

T. Bürgi*

Understanding the mechanism of voltage-sensitive SH fluorescent probes [PC-131]

Zhi Li, EPFL Lausanne

N. A. Correa Rojas, M. Eremchev, S. Roke*

Resolving the intrinsic heterogeneity of the splicing process of a group II intron through multiple pairwise labelling [PC-132]

Matteo Lisibach, University of Zurich

A. R. Sadiq, S. Zelger-Paulus*, R. K. O. Sigel*

One Ring to Rule Them All: Ultrafast Spectroscopy Study of Chiral Platina[n]helicenes with Circularly Polarized Emission [PC-133]

José Merkelj, University of Basel

L. M. Müller, M. Puppini, J. Crassous, M. J. Fuchter, M. Oppermann*

Real-time tracking of the ultrafast chirality and energy transfer in a chiral OLED complex with circularly-polarized luminescence [PC-134]

Livia Müller, University of Basel

F. Zinna, G. Pescitelli, M. Puppini, M. Oppermann*

How we can tackle the dielectric response around spherical polymer surface [PC-135]

Miroslava Nedyalkova, University of Fribourg

P. Loche, M. Lattuada

Controlled laboratory astrochemistry: Rotational-state-selected carbon reactions in space [PC-136]

Aswin Ravindran, University of Basel

L. Xu, T. Lejeune, S. Willitsch, J. Toscano*

New apparatus for single-photon Doppler-free VUV/XUV spectroscopy [PC-137]

Matthew Rayment, ETH Zurich

J. A. Agner, H. Schmutz, F. Merkt*

Conservation of wavefunction reflection parity in methane-surface scattering [PC-138]

Christopher Reilly, EPFL Lausanne

D. J. Auerbach, R. D. Beck*

Production of holmium radioisotopes for Targeted Radionuclide Therapy [PC-139]

Edoardo Renaldin, PSI
H. Zhang, S. Braccini, U. Köster, N. P. van der Meulen, R. Eichler, Z. Talip*

Photoinduced Dynamics of Symmetric π -Extended Aryl Acetylide Platinum Complexes with Isocyanides or Acyclic Diaminocarbenes: Symmetric or not? [PC-141]

Atzin Ruiz-Lera, University of Geneva
J. López-López, Y. Nguyen, T. Teets, R. Fernández-Terán*

Two level ordering in nano-rattles for optical properties [PC-142]

Antoine Scalabre, Fribourg University
K. M. Fromm*

Can increasing the size and flexibility of a molecule reduce decoherence? [PC-143]

Alan Scheidegger, EPFL Lausanne
N. V. Golubev, J. Vanicek*

Extraction and characterization of oleosomes from wheat germ. [PC-144]

Abinaya Subramaniyan, University of Fribourg
S. Salentinig*

Understanding the ultrafast charge transfer process in naphthalene diimide (NDI) based polymers and copolymers [PC-145]

Estefanía Sucre-Rosales, University of Geneva
S. Ye, Y. Bao, E. Vauthey*

State-preparation and quantum control of polyatomic molecular ions [PC-146]

Nanditha Sunil Kumar, University of Basel, Switzerland
P. Paliwal, M. Popov, S. Willitsch*

Comparing membrane potential imaging using water and FM4-64 dye as a probe [PC-147]

Iwona Swiderska, EPFL Lausanne
S. Lee, Z. Li, N. A. Correa, S. Roke*

Testing the ion funnel-to-IVAC system for fast chemistry experiments with superheavy elements [PC-148]

Georg Tiebel, Paul Scherrer Institut PSI/ETH Zurich
A. Bukowski, T. Cook, R. Dressler, R. Eichler, C. M. Folden III, J. Garcia, I. Haynes, D. Herrmann, Y. Ito, A. Kirkland, J. Mildon, T. Sato, E. Tereshatov, A. Vögele, V. Zakusilova, P. Steinegger*

Solvation Shifts the Band-Edge Position of Colloidal Quantum Dots by nearly 1 eV [PC-149]

Yan Vogel, ETH Zurich
L. Pham, M. Stam, R. Ubbink, M. L. Coote, A. Houtepen

Controlling Symmetry-Breaking Charge Separation in Pyrene Bichromophores [PC-150]

Johannes Wega, University of Geneva
K. Zhang, J. Lacour*, E. Vauthey*

Isotopic chirality and high resolution infrared spectroscopy of PFCl₂ [PC-151]

Gunther Wichmann, ETH Zurich
V. Horka-Zelenkova, A. Sieben, S. Albert, K. Keppler, G. Seyfang, J. Stohner, M. Quack*

Interfacial Inversion, Interference, and IR Absorption in Vibrational Sum Frequency Scattering Experiments [PC-152]

Li Zhang, EPFL Lausanne
S. Pullanchery, S. Roke*

In vivo ¹H MR Spectroscopy of bile acids from human gallbladder—Detection and quantification of metabolites after a lipid load [PC-153]

Yue Zhang, University of Bern
D. Kröll, G. Stirnimann, R. Wiest, P. Vermathen*

Single-photon superradiance in individual cesium lead halide quantum dots [PC-154]

Chenglian Zhu, ETH Zurich / EMPA
S. C. Boehme, L. G. Feld, A. Moskalenko, D. D. Dirin, R. F. Mahrt, T. Stöferle, M. I. Bodnarchuk, A. L. Efros, P. C. Sercel, G. Rainò*, M. V. Kovalenko*

Evaporation of Po from LBE-cooled reactors [PC-155]

Ivan Zivadinovic, Paul Scherrer Institute PSI, Villigen
J. Neuhausen*, P. Steinegger*

Tellurium speciation in vapors over Lead-Bismuth eutectic melts [PC-156]

Vladislav Zobnin, PSI / UniBern
J. Neuhausen*, R. Eichler*

**Materials Chemistry [Mat]
Poster Session**

Multicolor Emission with Photo-Switchable Cationic Pyridine-Pyrene (PyPy) for OLED [Mat-101]

Boopathi Achuthan, University of Fribourg
K. M. Fromm*

Electroactive naphthalimide and naphthalenediimide interlayers for inverted perovskite solar cells [Mat-102]

Konstantina Armadorou, EPFL Lausanne
G. AlSabeih, M. Najafov, F. T. Eickemeyer, L. Pfeifer, W. Niu, J. Milić*, M. Grätzel*

Diels-Alder Cycloaddition Polymerization for Porous Poly-phenylenes with Exceptional Gas Uptake Properties [Mat-104]

Timur Ashirov, University of Fribourg
P. W. Fritz, T. Yildirim*, A. Coskun*

From Chicken Feathers to Antimicrobial Peptides for Smart, Self-Disinfecting Nanocoating [Mat-105]

Amira Ben Mansour, HEIA Fribourg
J. Horner, S. Jansod, R. Marti*

Dynamically-bound Guanidinium-based Ligands for Lead Halide Perovskite Nanocrystals [Mat-106]

Yuliia Berezovska, ETH Zurich
S. Sabisch, C. Bernasconi, M. Bodnarchuk, D. Dirin, M. Kovalenko*

Optically actuated metallosupramolecular systems comprising opto-chemical transducers [Mat-107]

Luca Bertossi, Adolphe Merkle Institute, Fribourg
C. Weder*

A Colloidal Nanofactory for Solid-Liquid-Solid Nanoparticles [Mat-108]

Coline Boulanger, EPFL Lausanne
D. Arenas Esteban, K. Kumar, J. Leemans, P. P. Albertini, R. Buonsanti*, S. Bals*

Organic Additive Approach for the Interfacial Stabilization in Sulfide-based All-Solid-State Batteries [Mat-109]

Leonie Braks, University of Fribourg
A. Coskun*

Magnetic Metallocarbon Membranes – Towards a new semiconductor class [Mat-110]

Christian Bünzli, University of Basel
M. Mayor*

Novel synthesis and ligand design for lead-free halide perovskites. [Mat-111]

Ole Dressler, ETH Zurich
D. Dirin, M. Kovalenko*

Phonon-driven wavefunction localization promotes room-temperature, pure single-photon emission in large organic-inorganic lead-halide quantum dots [Mat-112]

Leon Feld, ETH Zurich
S. C. Boehme, S. Sabisch, N. Frenkel, N. Yazdani, V. Morad, C. Zhu, M. Svyrydenko, R. Tao, M. Bodnarchuk, G. Lubin, M. Kazes, V. Wood, D. Oron, G. Raino*, M. V. Kovalenko*

Designing inherently degradable epoxy resins around a carbohydrate core [Mat-113]

Maxime Hedou, EPFL/HEIA Fribourg
T. Nelis, L. Manker, M. Jones, R. Martinet, T. Borgmeyer, J. Staal, A. Demongeot, V. Michaud, F. Maréchal, J. Luterbacher*, R. Marti*

Sensitized triplet-triplet annihilation in nanostructured polymeric scintillators allows for pulse shape discrimination [Mat-114]

Xueqian Hu, Adolphe Merkle Institute
D. Rigamonti, I. Villa, L. Pollice, M. Mauri, A. Dal Molin, M. Tardocchi, F. Meinardi, C. Weder*, A. Monguzzi*

Supramolecular assembly induced fluorescence based on acridone oligomers [Mat-115]

Isabelle Kolly, University of Berne
S. M. Langenegger, R. Häner*, S. Liu*

Bronze-type niobium tungsten oxides: intricate structures for battery research [Mat-116]

Frank Krumeich, ETH Zurich
M. Wörle

Iron-carbohydrate complexes treating anaemia: understanding the dynamic Interactions with human blood serum [Mat-117]

Leonard Krupnik, Empa
B. F. Silva, J. Avaro, V. Lütz-Bueno, J. Kohlbrecher, A. Alston, R. Digigow, B. Flühmann, E. Philipp, P. Wick*, A. Neels*

Tuning crystal growth of 2D Covalent Organic Frameworks with acid catalysts [Mat-118]

Iris Landman, Northwestern University, Evanston, USA
A. Natraj, C. Pelkowski, W. R. Dichtel*

Triplet-Triplet Annihilation Upconversion with a New Class of UV Emitters [Mat-119]

Davide Lardani, Adolphe Merkle Institute, Fribourg
X. Hu, A. Monguzzi, C. Weder*

Chemical stability of gold-silica core-shell nanoparticles in biological media [Mat-120]

Wang Sik Lee, Adolphe Merkle Institute, Fribourg
P. Taladriz-Blanco, H. Lee, L. Hirschi-Ackermann, B. Rothen-Rutishauser, A. Petri-Fink*

Accelerated Reversible Conversion of Li_2S_2 to Li_2S by Spidroin Regulated Li^+ Flux for High-performance Li-Sulfur Batteries [Mat-121]

Mingliang Liu, University of Fribourg
A. Coskun*

Controlling the Magnetic Properties of the van der Waals Multiferroic Crystals $\text{Co}_{1-x}\text{Ni}_x\text{I}_2$ [Mat-122]

Anastasiia Lukovkina, University of Geneva
E. Giannini*, S. A. López-Paz, C. Besnard, L. Guenee, F. O. von Rohr*

S-Mediated Interactions in Hybrid Perovskite Photovoltaics [Mat-123]

Weifan Luo, University of Fribourg
S. Kim, J. Milić*

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