

SCS Fall Meeting 2022

Thursday, September 8, 2022, 09.15-18.30h

University of Zürich, Irchel Campus

Plenary Talks

- **Dr. Theodoro Laino**, IBM Research, Zürich, member of the Sandmeyer Award team 2022
- **Prof. Xile Hu**, EPFL Lausanne, Swiss Green & Sustainable Chemistry Award winner 2022
- **Dr. Bernd Kuhn**, F. Hoffmann-La Roche AG, SCS Senior Industrial Science Award winner 2022
- **Prof. Antonio Togni**, ETH Zürich, Paracelsus Award winner 2022

Parallel Session and Poster Session Topics

- Analytical Sciences
- Catalysis Science & Engineering
- Computational Chemistry
- Chemistry and the Environment
- Inorganic & Coordination Chemistry
- Medicinal Chemistry & Chemical Biology
- Organic Chemistry
- Physical Chemistry
- Polymers, Colloids & Interfaces

Online registration is possible until September 2, 2022

On-site registration is possible but be prepared for waiting time.

Fall Meeting 2022 graphic: Interpretation of the "arms race" between bacteria and antibiotics, Erik Jung, University of Zürich



University of
Zürich ^{UZH}



SCS
Swiss Chemical
Society

WELCOME TO THE SCS FALL MEETING 2022 OF THE SWISS CHEMICAL SOCIETY



Prof. Roger Alberto



Dr. Hans Peter Lüthi

On behalf of the Organizing Committee, the Board Members of all involved SCS Networks, and the University of Zürich Department of Chemistry, we welcome you to the 2022 Fall Meeting!

This is a moment we have long been waiting for: The Fall Meeting is back as an on-site event! After two virtual events operated out of the “control center” at the University of Bern^[1], we will now be meeting again in person at the beautiful Irchel Campus.

The Fall Meeting program and structure has not changed: After the Welcome and Opening, we will be enjoying Award Lectures, followed by the nine thematic parallel sessions, the platforms for students to present their research. During the Lunch Break the participants will have the opportunity to visit the Poster Sessions and the Commercial Exhibition. Now, the drinks and sandwiches will be real, and the interaction with the poster presenters will again be face-to-face, i.e. no Gather.Town virtual environment. In the afternoon, there is the second round of parallel sessions and Award Lectures. The meeting ends with the announcement of the winners of the „Helvetica Prize of the SCS“, and the Award Ceremony, honoring the Best Oral and Best Poster Presenters. This is one of the best-endowed Award Programs of its kind, and the Ceremony is always one of the highlights of a very long and intense day.

The Fall Meeting is the most important platform for the next generation of chemists in Switzerland. For many, it is the first occasion to meet the community and to present their accomplishments outside the walls of their laboratories. More than 450 students submitted an abstract. Overall, the presentations of senior lecturers included, there will be around 100 oral presentations. At the Poster Session, 350 posters will be open for discussion, creating this wonderful, sizzling atmosphere of vivid exchange between participants.

We gratefully acknowledge the generous support of our sponsors, many of which have supported us for year. The University of Zürich Department of Chemistry is again our wonderful host. We thank all the members of the Organizing Committee for setting up attractive session programs. Finally, we would like to thank the fifty student helpers of the University of Zürich and ETH Zürich. We invite you to browse through the program and look forward to meeting you at the Irchel Campus.

Prof. Roger Alberto
Co-Chair of the Organizing Committee

Dr. Hans Peter Lüthi
Co-Chair of the Organizing Committee

[1] Hans Peter Lüthi, Silvio Decurtins, David Spichiger, and Céline Wittwer, ‘Fall Meeting 2020: A Success Story Based on ‘Plan B’, *Chimia* 2020, 74, 831–832

PROGRAM OVERVIEW, THURSDAY, 8TH SEPTEMBER 2022

Interactive program incl. abstracts of all lectures, talks and poster abstracts on fm22.scg.ch

Time	Program Item
08.30	Registration and welcome coffee
09.15	Welcome and conference opening <i>Prof. Roger Alberto</i> , University of Zurich, Co-Chair of the SCS Fall Meeting 2022 <i>Prof. Elisabeth Stark</i> , Vice President Research, University of Zurich
Morning Plenary Session (Award Lectures) , Chair: Christian Bochet	
09.30	Sandmeyer Award Lecture 2022 <i>Dr. Theodoro Laino</i> , IBM Research Europe, Zurich «Fueling the Digital Chemistry Revolution with Language Models»
10.00	Swiss Green & Sustainable Chemistry Award Lecture 2022 <i>Prof. Xile Hu</i> , EPFL Lausanne «Cooperative Molecular, Bio-, and Electrocatalysis»
10.30	Short break
Morning Parallel Sessions	
10.45	Invited/Sponsored Lecture (30 min) and Short Talks (15 min) Topics: Analytical Sciences, Catalysis Science & Engineering, Computational Chemistry, Chemistry and the Environment, Inorganic & Coordination Chemistry, Medicinal Chemistry & Chemical Biology, Organic Chemistry, Physical Chemistry, Polymers, Colloids & Interfaces
Lunch Break and Poster Session	
12.30	Virtual Poster Sessions (same topics as the parallel lecture sessions) Commercial Exhibition Visit the booths and learn about the latest developments from our partners. Participate in the exhibitor challenge and get the chance to win 1x 100 and 2x 50 CHF in cash.
13.30	General Assembly of the youngSCS 2022 Lead: Lluç Farrera Soler, President youngSCS
Afternoon Parallel Sessions	
14.30	Invited/Sponsored Lecture (30 min) and Short Talks (15 min) Topics: Analytical Sciences, Catalysis Science & Engineering, Computational Chemistry, Chemistry and the Environment, Inorganic & Coordination Chemistry, Medicinal Chemistry & Chemical Biology, Organic Chemistry, Physical Chemistry, Polymers, Colloids & Interfaces
16.15	Short break
Afternoon Plenary Session (Award Lectures) , Chair: Christian Bochet	
16.30	SCS Senior Industrial Science Award Lecture 2022 <i>Dr. Bernd Kuhn</i> , F. Hoffmann-La Roche AG «Details Matter in Structure-based Drug Design»
17.00	Paracelsus Award Lecture 2022 <i>Prof. Antonio Togni</i> , ETH Zurich «For the Sake of Making Molecules»
SCS Announcements and Ceremony Session	
17.45	SCS Announcements Helvetica Prize of the Swiss Chemical Society 2022 (best published papers of PhD/Postdocs 2021/22)
18.00	Best Oral Presentation Awards (sponsored by Metrohm) Dipl. Ing. Markus Steinke, Metrohm AG Best Poster Presentation Awards (sponsored by DSM) Dr. Werner Bonrath, DSM Nutritional Products Ltd.
18.30	End of the conference

GENERAL INFORMATION

Date: September 8, 2022, 08.30 – 18.30h
 Location: Irchel Campus, University of Zurich
 Host: University of Zurich
 Website: <https://fm22.scg.ch/>

Conference Secretariat

Swiss Chemical Society
 Haus der Akademien
 Laupenstrasse 7, Postfach
 3001 Bern
info@scg.ch

Organizing Committee

Chairs

- Prof. Roger Alberto, University of Zurich
ariel@chem.uzh.ch
- Dr. Hans Peter Lüthi, ETH Zurich and SCS Foundation
luethi@scg.ch

Members of the Extended Organizing Committee

Analytical Sciences

- Dr. Hanspeter Andres, Federal Institute of Metrology, METAS
- Prof. Eric Bakker, University of Geneva
- Dr. Ksenia Groh, Eawag Dübendorf

Catalysis Sciences & Engineering

- Prof. Martin Albrecht, University of Bern
- Prof. Jeroen A. van Bokhoven, ETH Zurich and PSI Villigen

Computational Chemistry

- Prof. Jürg Hutter, University of Zurich
- Prof. Jeremy Richardson, ETH Zurich

Inorganic & Coordination Chemistry

- Prof. Roger Alberto, University of Zurich
- Prof. Murielle Delley, University of Basel
- Prof. Marinella Mazzanti, EPF Lausanne

Organic Chemistry

- Prof. Sascha Hoogendoorn, University of Geneva
- Prof. Michal Juríček, University of Zurich
- Prof. Francesca Paradisi, University of Bern

Medicinal Chemistry & Chemical Biology

- Dr. Dennis Gillingham, University of Basel
- Prof. Jean-Louis Reymond, University of Bern
- Dr. Antonia Stephan, F. Hoffmann-La Roche AG

Physical Chemistry

- Prof. Thomas Bürgi, University of Geneva
- Prof. Cornelia Palivan, University of Basel

Plymers, Colloids & Interfaces

- Prof. Esther Amstad, EPFL Lausanne
- Dr. Dorina Opris, Empa Dübendorf
- Prof. Paolo Arosio, ETH Zurich

Chemistry and the Environment

- Prof. Kathrin Fenner, Eawag Dübendorf und University of Zurich
- Dr. Jutta Hellstern, F. Hoffmann-La Roche AG

Participation Fees

Fees for presenters (poster or talk)

- SCS Members: free of charge (by convention the first name in the abstract authors' 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 15 will have to pay the fees by credit card during the registration process.



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

Coffee Breaks and Lunch

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

There is also the possibility to have lunch at your own expense in the cafeterias and restaurants on the Irchel campus next to the conference venue.

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 files
- pdf-file download of single abstracts
- Extensive search functionalities

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.

The screenshot displays the SCS Fall Meeting 2022 website interface. At the top, it shows the event title and location. Below is a navigation menu with numbered callouts: 1 (Home), 2 (Abstract Upload), and 3 (Program). The main content area is divided into two sections. On the left, a 'Schedule of Fall Meeting 2022' table lists sessions from 09:15 to 12:00, including 'Welcome and Conference Opening', 'Fusing the Digital Chemistry Revolution with Language Models', 'Cooperative molecular, bio- and electrocatalysis', 'Coffee Break', 'Using Proximal Cations to Install Internal Electric Fields in Transition Metal Complexes', 'Exploiting Cobalt(III) Amide Complexes in Degronative Fluoroaromatic Molecules', 'Synthesis, Structural Heterocyclic β -Oxal', 'Cation assisted binuclear', and '(Re)investigating ternary rare-earth β -diketonates complexes'. On the right, an abstract preview for 'Exploiting Cobalt(III) Amide Complexes in Degronative Metalation of Fluoroaromatic Molecules' is shown, featuring a chemical structure and a list of references.

BEST PRESENTATION AWARDS

The organizers are proud of the very attractive presentation award program. More than CHF 42'000 CHF in total are given to the winners in cash, travel grants or free publication opportunities in the Junior Laureates issue of CHIMIA 4/2023.

We would like to address our recognition and thanks to the Metrohm Foundation and to DSM Nutritional Products Ltd., who have partnered the presentation award program for many years.

Best Oral Presentation Award

The award is sponsored by Metrohm.



The prize is given for the 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: 18.00h in the plenary lecture room.

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 presented by Dipl. Ing. Markus Steinke, Executive Vice President Marketing at Metrohm International Headquarters, Herisau.

Best Poster Presentation Award

The award is sponsored by DSM.



The prizes are given for the best posters of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 18.15h in the plenary lecture room.

Prize for the winner of each of the nine poster sessions

- Cash contribution of CHF 250.
- 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

- cash contribution of CHF 200 (1-3 prizes, based on the number of presented posters in the respective session)

The prizes are sponsored by DSM Nutritional Products and will be presented by Dr. Werner Bonrath, Senior Researcher at DSM Nutritional Products Ltd., Basel.



Covers of the 2020–2022 Junior Laureates Issues

HELVETICA PRIZE OF THE SWISS CHEMICAL SOCIETY 2022



Helvetica and the Swiss Chemical Society are proud to award the winners of the Helvetica Prize 2022 of the Swiss Chemical Society for the best published papers of PhD/Postdocs 2021/22 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, Managing Editor of Wiley-VHCA will honor the winners who will present their papers in a 3min short presentation.

1st Prize: **Jordan De Jesus Silva**, ETH Zurich

Corresponding author: Christophe Copéret

«Development and Molecular Understanding of a Pd-Catalyzed Cyanation of Aryl Boronic Acids Enabled by High-Throughput Experimentation and Data Analysis»

DOI: <https://doi.org/10.1002/hlca.202100200>

2nd Prize: **Weilong Liu** and **Emma E. Watson**, University of Geneva. Corresponding author: Nicolas Winssinger

«Photocatalysis in Chemical Biology: Extending the Scope of Optochemical Control and Towards New Frontiers in Semisynthetic Bioconjugates and Biocatalysis»

DOI: <https://doi.org/10.1002/hlca.202100179>

Winners of the Best Presentation Awards 2021



SPONSORS AND SUPPORTERS OF THE SCS FALL MEETING

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 SUPPORTERS AND GENERAL SPONSORS



AWARD SPONSORS



Best Oral Presentation Award



Best Poster Presentation Award



Helvetica Prize of the Swiss Chemical Society

ENDOWMENTS OF PARALLEL SESSIONS



Analytical Sciences



Catalysis Science & Engineering



Chemistry and the Environment



Computational & Theoretical Chemistry



Inorganic & Coordination Chemistry



Medicinal Chemistry & Chemical Biology



Organic Chemistry



Polymers, Colloids & Interfaces

COMMERCIAL EXHIBITORS



PLENARY SESSIONS

Award Lectures in the Plenary Sessions

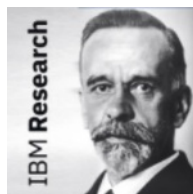
Chair: Prof. Christian Bochet, University of Fribourg,
SCS President

Sandmeyer Award Lecture 2022

«Fueling the Digital Chemistry
Revolution with Language Models»
[PS-001]

September 8, 2022, 9.30h

Dr. Teodoro Laino, IBM Research Europe



The SCS honors **Alain Vaucher, Daniel Probst, Philippe Schwaller, Theophile Gaudin, Teodoro Laino, Matteo Manica, Alessandra Toniato, Federico Zipoli, Antonio Cardinale, Alessandro Castrogiovanni, Heiko Wolf, Aleksandros Sobczyk, Joppe Geluykens**, from the RXN for Chemistry Project Team from IBM Research for their important scientific breakthrough in the digitalization of synthetic organic chemistry that helps to improve digital work-flows with state-of-the-art machine learning technologies.

Swiss Green & Sustainable Chemistry Award Lecture 2022

«Cooperative Molecular, Bio-, and Electrocatalysis» [PS-002]
September 8, 2022, 10.00h

Prof. Xile Hu
EPFL Lausanne



Xile is awarded for his outstanding, interdisciplinary research program to develop catalysis for sustainable synthesis of added-value chemicals and for cost-effective production of solar and electric fuels.

SCS Senior Industrial Science Award Lecture 2022

«Details Matter in Structure-based Drug Design» [PS-003]
September 8, 2022, 16.30h

Dr. Bernd Kuhn
F. Hofmann-La Roche Ltd.

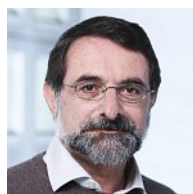


Awarded in recognition of his groundbreaking achievements over the past two decades, bringing together novel computational approaches and medicinal chemistry knowledge that led to new drug designs and scientific discoveries that have had tremendous impact on small molecule discovery projects.

Paracelsus Prize Lecture 2022

«For the Sake of Making Molecules» [PS-004]
September 8, 2022, 17.00h

Prof. Antonio Togni
ETH Zurich



The award is given to honor his groundbreaking contributions to organic, inorganic, organometallic chemistry and catalysis both in industry and academia as well as for his inspiring approaches to teaching and education.

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
PI	Polymers Colloids & Interfaces
PS	Plenary Session

[XY-011]...[XY-017]	Morning parallel session lectures
[XY-021]...[XY-027]	Afternoon parallel session lectures
[XY-101]...[XY-199]	Posters presentations

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 1x 100.00 CHF.
Cards with at least one full column or one full row take part in the draw of 2x 50.00 CHF.

The drawing takes place on September 8, at 18:00h.

PARALLEL SESSIONS

Analytical Sciences [AS]

Session Endowment: Mettler Toledo



Chairs: Dr. Ksenia Groh, Eawag
Dr. Hanspeter Andres, METAS

- 10:45 **Relevance of solid forms and its implication on the performance of pharmaceutical drug products [AS-011]**
Arnaud Grandeury, Novartis Pharma AG
- 11:15 **Aptapaper – An aptamer-based glass fiber paper platform for rapid upconcentration and detection of small molecules [AS-013]**
Sandra Martínez-Jarquín, ETH Zurich
A. Begley, Y. Lai, G. Bartolomeo, A. Pruška, C. Rotach, R. Zenobi
- 11:30 **Temperature-Controlled Electrospray: A Window into Solution Thermochemistry of Non-Canonical Nucleic Acid Complexes [AS-014]**
Adam Pruška, ETH Zurich
J. A. Harrison, A. Marchand, A. Granzhan, R. Zenobi
- 11:45 **Advancing Cyclic Ion Mobility Mass Spectrometry Methods for Studying Biomolecules: Towards the Analysis of Mega Dalton Protein Aggregates [AS-015]**
Julian Harrison, ETH Zurich
A. Pruška, R. Zenobi
- 12:00 **Quantification of endotoxins in bacterial bioreactor samples and correlation of the endotoxin content to optical density and dry cell weight [AS-016]**
Anika Hoffmann, HES-SO Valais-Wallis
K. Pacios, R. Mühlemann, R. Daumke, B. Frank, F. Kalman
- 12:15 **Combining Activity Profiling with Advanced Annotation to Accelerate the Discovery of Natural Products Targeting Oncogenic Signaling in Melanoma [AS-017]**
Eliane Garo, University of Basel
T. Hell, A. Rutz, L. Dürr, M. Dobrzyński, J. K. Reinhardt, O. Pertz, M. Hamburger, J. Wolfender, E. Garo
-
- 14:30 **Does digitalization in R&D slow down innovation and take away flexibility? What is the risk of ignoring the benefits of digitalization? [AS-021]**
Christoph Jansen, Mettler Toledo GmbH
- 15:00 **Influence of Chlorinating Agents on the Formation of Stable Biomarkers in Hair for the Retrospective Verification of Exposure [AS-023]**
Severin Martz, University of Fribourg
M. Wittwer, C. Tan-Lin, M. Brackmann, C. Bochet, C. Curty
- 15:15 **Rapid Spectroscopic Detection of Volatile Organic Compounds With Widely Electrically Tuneable Quantum-Cascade Lasers [AS-024]**
Miloš Selaković, Empa
R. Brechbühler, P. Scheidegger, H. Looser, A. Kupferschmid, B. Tuzson, L. Emmenegger
- 15:30 **Visualizing Surface Phase Separation in PS-PMMA Polymer Blends at the Nanoscale using Tip-Enhanced Raman Spectroscopy [AS-025]**
Dušan Mđrenović, ETH Zurich
D. Abbott, V. Mougél, W. Su, N. Kumar, R. Zenobi
- 15:45 **Pure Isotropic Proton Solid State NMR [AS-026]**
Bruno Simões de Almeida, EPFL Lausanne
P. Moutzouri, D. Torodii, M. Cordova, L. Emsley
- 16:00 **OCompressed Sensing for Rapid Signal Retrieval in X-ray Absorption Spectroscopy [AS-027]**
Yousuf Hemani, Empa
K. Koch, D. Bleiner

Catalysis Sciences & Engineering [CE]

Session Endowment: Chemspeed



Chairs: Prof. Martin Albrecht, University of Bern
Prof. Jeroen A. van Bokhoven, ETHZ/PSI Villigen

- 10:45 **Catalytic Methods for the Construction of Halogen-Functionalized Organic Compounds with Application to Late-Stage Functionalizations [CE-011]**
Belén Martín-Matute, Stockholm University
- 11:15 **Catalytic Carbochlorocarbonylation of Unsaturated Hydrocarbons via C–COCl Bond Cleavage [CE-013]**
Elliott Denton, ETH Zurich
Y. H. Lee, S. Roediger, P. Boehm, M. Fellert, B. Morandi
- 11:30 **Oxygen Atom Transfers Catalyzed by Cobalt Sulfide [CE-014]**
Vanessa Wyss, University of Basel
M. F. Delley
- 11:45 **Iridium complexes bearing O-functionalized PYE ligands for efficient formic acid dehydrogenation [CE-015]**
Nicolas LENTZ, University of Bern
M. Albrecht
- 12:00 **Tools for Predicting the Activity of Immobilized Frustrated Lewis Pair Catalysts [CE-016]**
Shubhajit Das, EPFL Lausanne
R. Laplaza, J. T. Blaskovits, C. Corminboeuf
- 12:15 **Non-oxidative Coupling of Methane with Transition-Metal Carbides: Mechanistic Revelation of the Role of Carbide Carbon [CE-017]**
Seraphine Zhang, ETH Zurich
Q. Pessemesse, L. Lätsch, K. Engel, A. van Bavel, A. Horton, P. Payard, C. Copéret
-
- 14:30 **What is more important to enable efficient cyber-physical systems – digital twins or the degree of automation in R&D labs? [CE-021]**
Rolf Gueller, Chemspeed Technologies AG
- 15:00 **Operando X-ray spectroscopy revealed the key role of the Pt-FeOx catalytic interface in preferential CO oxidation [CE-023]**
Ilia Sadykov, Paul Scherrer Institute (PSI)
V. L. Sushkevich, F. Krumeich, R. J. Nuguid, J. A. van Bokhoven, M. Nachtegaal, O. V. Safonova
- 15:15 **OER Catalyst's Transport Layer Matters: Stability Comparison Between C Based GDL and Ti Based PTL [CE-024]**
Aline Bornet, University of Bern
S. Pitscheider, E. Bertheussen, C. M. Pedersen, A. Maletzko, N. Sesej, G. K. Wiberg, C. Kallesoe, J. Melke, M. Arenz
- 15:30 **Bimetallic CoPt Nanoparticles for the Dry Reforming of Methane: Understanding Structure-Performance Relationships [CE-025]**
David Niedbalka, ETH Zurich
P. M. Abdala, N. Zimmerli, C. R. Müller
- 15:45 **Atomically precise design of bimetallic Au-Ru and Ru-Pt low nuclearity catalysts via carbon host functionalization [CE-026]**
Vera Giulimondi, ETH Zurich
S. K. Kaiser, A. Ruiz-Ferrando, A. J. Martín, S. Büchele, F. Krumeich, A. H. Clark, N. López, J. Pérez-Ramírez
- 16:00 **Dynamics of nanoparticle motion and metal-oxide support in redox-reactive gases [CE-027]**
Hannes Frey, ETH Zurich
A. Beck, X. Huang, J. A. van Bokhoven, M. G. Willinger

Computational and Theoretical Chemistry [CC]

Session Endowment: Syngenta

Chairs: Prof. Jürg Hutter, University of Zurich
Prof. Jeremy Richardson, ETH Zurich

- 10:45 **Fluctuations Beyond Chemical Imagination in Liquid Water [CC-011]**
Ali Hassanali, The International Center for Theoretical Physics (ICTP), Trieste
- 11:15 **Enzeptional: enzyme optimization via a generative language modeling-based evolutionary algorithm [CC-013]**
Yves Gaetan Nana Teukam, Eindhoven University of Technology
M. Manica, F. Grisoni, T. Laino
- 11:30 **Predicting chemical toxicity through machine learning [CC-014]**
Christoph Schür, Eawag Dübendorf
L. Gasser, J. Wu, F. Perez-Cruz, K. Schirmer, M. Baity-Jesi
- 11:45 **The Spectrum of Approximated Hamiltonian Matrices Representations (SPA^{HM}) [CC-015]**
Ksenia Briling, EPFL Lausanne
Y. Calvino Alonso, A. Fabrizio, C. Corminboeuf
- 12:00 **Pathfinder – A Route Planner for Chemical Reaction Networks [CC-016]**
Paul Türtcher, ETH Zurich
M. Reiher
- 12:15 **Mechanistic investigations at the alumina/water interface [CC-017]**
Carine Michel, École Normale Supérieure of Lyon
-
- 14:30 **Digital Chemistry at Syngenta: from academic labs to industrial applications [CC-021]**
Arndt R. Finkelmann, Syngenta Crop Protection
- 15:00 **Electric Field Gradient calculation within Frozen-Density Embedding Theory [CC-023]**
Yann Gimbal-Zofka, University of Geneva
T. Wesolowski
- 15:15 **Random projections in computational quantum mechanics [CC-024]**
Aleksandros Sobczyk, IBM Research Europe
T. Laino, M. Luisier
- 15:30 **Search for long-lasting electronic coherence using on-the-fly ab initio semiclassical dynamics [CC-025]**
Alan Scheidegger, EPFL Lausanne
J. Vaníček, N. Golubev
- 15:45 **Recent Advances in the Development of Accurate Forcefields for Modelling Phase Stabilities in Hybrid Halide Perovskites [CC-026]**
Mathias Dankl, EPFL Lausanne
U. Röthlisberger
- 16:00 **Copper-Based Catalysts for COX Hydrogenation To Methanol – Metadynamics Bridges the Pressure and Material Gap [CC-027]**
Andreas Müller, ETH Zurich
J. L. Alfke, A. Comas-Vives, O. Safonova, C. Copéret

Chemistry and the Environment [EV]

Session Endowment: DSM

Chairs: Dr. Isabelle Worms, University of Geneva
Dr. Thomas Bucheli, Agroscope ETH Zurich

- 10:45 **Oxidation processes for micropollutant abatement: An Eldorado for environmental chemists [EV-011]**
Urs von Gunten, Eawag, Dübendorf
- 11:15 **Combination of advanced analytical tools with toxicological assays promote the understanding of transformation reactions occurring during wastewater ozonation [EV-013]**
Tarek Manasfi, Eawag, Dübendorf
C. McArdell, J. Hollender, U. von Gunten, T. Manasfi
- 11:30 **Laboratory validation of a laser absorption spectrometer for balloon-borne measurements of upper air water vapor [EV-014]**
Simone Brunamonti, Empa
M. Graf, T. Bühlmann, L. Emmenegger, B. Tuzson
- 11:45 **In situ quantification of Cobalt and Nickel in natural waters using innovative chemical sensors [EV-015]**
Nicolas Layglon, University of Geneva
S. Creffield, E. Bakker, M. Tercier-Waeber
- 12:00 **Acidity of expiratory aerosols controls the infectivity of airborne influenza virus and SARS-CoV-2 [EV-016]**
Aline Schaub, EPFL Lausanne
I. Glas, L. Klein, S. David, W. Hugentobler, A. Nenes, U. Krieger, S. Stertz, T. Peter, T. Kohn
- 12:15 **Adsorption and transport of water-soluble, biodegradable polymers in soils: Process elucidation using experimental model systems [EV-017]**
Kevin Kleemann, ETH Zurich
M. Sander
-
- 14:30 **Green Processes of the Future - Sustainability along the value chain [EV-021]**
Christian Schäfer, DSM Nutritional Products Ltd.
- 15:00 **Investigating the Applicability of Laboratory derived Toxicokinetics to the Field [EV-023]**
Benedikt Lauper, Eawag
E. Anthamatten, S. Käslin, J. Raths, M. Arlos, J. Hollender
- 15:15 **Organ-specific biotransformation in salmonids: insight into enzyme kinetics and micro-pollutant clearance [EV-024]**
Marco Franco, Eawag
R. Schönenberger, J. Hollender, K. Schirmer
- 15:30 **enviRule: An End-to-end System for Automatic Extraction of Reaction Patterns from Environmental Contaminant Biotransformation Pathways [EV-025]**
Kunyang Zhang, University of Zurich
K. Fenner
- 15:45 **Development and scale-up of bio-based solvents by carbohydrate functionalization [EV-026]**
Anastasiia Komarova, EPFL Lausanne
J. Luterbacher
- 16:00 **Decentralized solar ammonia: performance targets for environmental and economic benefits [EV-027]**
Sebastiano D'Angelo, ETH Zurich
A. J. Martín, D. Freire Ordóñez, S. Cobo, G. Guillén Gosálbez, J. Pérez-Ramírez

Inorganic & Coordination Chemistry [IC]

Session Endowment: Sika


 Chairs: Prof. Murielle Delley, University of Basel
 Prof. Marinella Mazzanti, EPFL Lausanne

- 10:45 **Using Proximal Cations to Install Internal Electric Fields in Transition Metal [IC-011]**
 Jenny Yang, University of California, Irvine
 N. Leonard, T. Chantarojsiri
- 11:15 **Exploiting Cobalt(II) Amide Complexes in Deprotonative Metalation of Fluoroaromatic Molecules [IC-013]**
 Alessandra Logallo, University of Bern
 E. Hevia
- 11:30 **Synthesis, Structure, Reactivity and Catalytic Activity of Octahedral Heteroleptic β -Diketonate Complexes of Molybdenum [IC-014]**
 Fabio Maserio, ETH Zurich
 V. Mougel
- 11:45 **Cation assisted binding and cleavage of dinitrogen by uranium complexes [IC-015]**
 Nadir Jori, EPFL Lausanne
 R. Scopelliti, I. Živković, T. Rajeshkumar, A. Sienkiewicz,
 L. Maron, M. Mazzanti
- 12:00 **(Re)investigating ternary rare-earth β -diketonates complexes: making new insights out of old ones [IC016]**
 Amina Benchohra, University of Geneva
 L. Guénée, C. Bernard, C. Piguet
- 12:15 **Synthesis and Characterization of an Artificial Iron-Sulfur Metalloenzyme [IC-017]**
 Valerie Waser, University of Basel
 M. Mukherjee, N. V. Igareta, T. R. Ward
-
- 14:30 **Toward CO₂-reduced Binders: Limestone Calcined Clay Cements with Improved Workability [IC-021]**
 Patrick Juilland, Sika Technology AG
- 15:00 **Anticancer rhenium di- and tricarbonyl complexes and synthesis of new α -diimine rhenium dicarbonyl complexes [IC-023]**
 Kevin Schindler, University of Fribourg
 K. Schindler, J. Delasoie, J. Rossier, A. Crochet, A. Pavic,
 F. Zobi
- 15:15 **[^{99m}Tc(η^6 -pharm)]⁺ synthesis with direct labelling of pharmaceuticals in water [IC-024]**
 Federica Battistin, University of Zurich
 Q. Nadeem, O. Blacque, R. Alberto
- 15:30 **Metal Amidinate Precursors for Easy Access to Supported Nanoparticles [IC-025]**
 Christian Ehinger, ETH Zurich
 C. Copéret
- 15:45 **Molecular controllable cubane oxo cluster catalysts and their dynamic role on photoanodes for water oxidation [IC-026]**
 Shangkun Li, University of Zurich
 W. Marks, H. Chen, G. R. Patzke
- 16:00 **β -X vs. β -H Elimination. Selection Rules for Chemoselectivity Enabled by Mechanistic Studies† [IC-027]**
 Michael Bogdos, ETH Zurich
 O. Stepanović, A. Bismuto, M. Luraschi, B. Morandi

Medicinal Chemistry & Chemical Biology [MC]

Session Endowment: idorsia


 Chairs: Dr. Antonia Stephan, F. Hofmann-La Roche
 Dr. Dennis Gillingham, University of Basel
 Prof. Jean-Louis Reymond, University of Bern

- 10:45 **General Assembly of the SCS Division of Medicinal Chemistry & Chemical Biology 2022 [MC-011]**
 Jean-Louis Reymond, University of Bern
- 11:00 **Discovery and characterization of ACT-284069, a double prodrug of the P2Y₁₂ receptor antagonist selatogrel [MC-012]**
 Eva Caroff, Idorsia Pharmaceuticals Ltd
 F. Hubler, C. Gnerre, A. Treiber
- 11:15 **Exploring Bicyclic Diamines as Drug Scaffolds [MC-013]**
 Aline Carrel, University of Bern
 J. L. Reymond
- 11:30 **PET Imaging of Cannabinoid Type 2 Receptors – Discovery of [¹⁸F]RoSMA-18-d₆ [MC-014]**
 Luca Gobbi, F. Hoffmann-La Roche AG
- 11:45 **YAP-TEAD protein protein interaction inhibitors. Discovery of the first class of small molecules efficiently disrupting the interaction by virtual screening and structure-based design [MC-015]**
 Pascal Furet, Novartis AG
- 12:00 **Bioactive Polymersomes Targeting Cancer-Associated Fibroblasts for Anticancer Therapy [MC-016]**
 Dimitri Hürlimann, University of Basel
 M. Skowicki, M. Kyropoulou, A. S. Gheata, W. P. Meier,
 S. Gerber-Lemaire, C. G. Palivan
- 12:15 **Comparative metabolomics reveals the gene function of *kat-1* in *C. elegans* [MC-017]**
 Marie-Désirée Scheidt, University of Neuchâtel
 S. Bandi, S. von Reuss
-
- 14:30 **Cyclic Tetrapeptides: Novel Remedy for Lead Poisoning [MC-021]**
 Tagwa Mohammed, University of Zurich
 C. M. Meier, L. Rulíšek, M. S. Shoshan
- 14:45 **A rational and systematic approach to PROTACs development: identification of CBP/EP300 degraders [MC-022]**
 Leonardo Palaferri, University of Zurich
 I. Cheng-Sánchez, K. Gosselé, C. Nevado
- 15:00 **Achiral Supercritical fluid Chromatography (SFC) for the Purification of Pharmaceuticals [MC-023]**
 John Reilly, Novartis
- 15:15 **Single-molecule profiling of PRC1 ubiquitination dynamics in defined chromatin states [MC-024]**
 Alexandra Teslenko, EPFL Lausanne
 B. Fierz
- 15:30 **Synthesis of short peptides in 384-well plates for generating large libraries of macrocyclic compounds [MC-025]**
 Mischa Schüttel, EPFL Lausanne
 E. Will, C. Heinis
- 15:45 **Discovery of RG6006, a Tethered Macrocyclic Peptide Targeting *Acinetobacter baumannii* [MC-026]**
 Patrizio Mattei, F. Hoffmann-La Roche AG
- 16:00 **Development of HLB-0532259: A First-in-Class Chemical Degradator of Aurora Kinase A and the N-Myc Transcription Factor [MC-027]**
 Daniel Harki, University of Minnesota
 J. Tang, R. Moorthy, Ö. Demir, Z. D. Baker, J. A. Naumann,
 K. F. Jones, M. J. Grillo, E. S. Haefner

Organic Chemistry [OC]

Session Endowment: Janssen/Cilag

Chairs: Prof. Francesca Paradisi, University of Bern
Prof. Sascha Hoogendoorn, University of Geneva

- 10:45 **Hydrogen Atoms in Halogen-Atom Transfer [OC-011]**
Daniele Leonori, RWTH Aachen University
- 11:15 **Nickel-Catalyzed Asymmetric Synthesis of α -Arylbenzamides [OC-013]**
Sergio Cuesta-Galisteo, University of Zurich
J. Schörgenhumer, X. Wei, E. Merino, C. Nevado
- 11:30 **Amino-oxetanes as amide isosteres by an alternative defluorosulfonylative coupling of sulfonyl fluorides [OC-014]**
Juan Rojas, Imperial College London
R. A. Croft, A. J. Sterling, E. L. Briggs, D. Antermite, D. C. Schmitt, A. J. White, C. Choi, J. J. Mousseau, J. A. Bull
- 11:45 **Development of New Synthetic Approaches Towards Acridinium Salts and Their Applications [OC-015]**
Valeriia Hutskalova, University of Basel
C. Sparr
- 12:00 **Benzodiazepinoindoles: Chiral Polycyclic Platforms for Various Applications [OC-016]**
Nidal Saleh, University of Geneva
J. Lacour, N. Saleh, J. Lacour
- 12:15 **Harnessing Deep Eutectic Solvents for Polar Organometallic Additions to α,β -unsaturated Ketones in Air [OC-017]**
Andrew Platten, University of Bern
E. Hevia
-
- 14:30 **The Chemical Development of Adafosbuvir, a Nucleoside Phosphoramidate Prodrug for the Treatment of Hepatitis C Infection [OC-021]**
Trung Cao, Janssen Pharmaceutica
S. Wagschal, S. Lemaire
- 15:00 **Non-innocent electrophiles unlock exogenous base-free coupling reactions [OC-023]**
Georgios Toupalas, ETH Zurich
B. Morandi
- 15:15 **Kinetically controlled stereoselective access to branched 1,3-Dienes by Ru-Catalyzed remote Conjugative Isomerization [OC-024]**
Simone Scaringi, University of Geneva
C. Mazet
- 15:30 **Palladium(0)-Catalyzed Enantioselective C(sp²)-H Arylation of (Hetero)arenes [OC-025]**
Shu-Min Guo, University of Basel
S. Huh, O. Baudoin
- 15:45 **Chemodivergent Asymmetric Synthesis via Catalytically Formed Chiral Auxiliary [OC-026]**
Mikus Purins, EPFL Lausanne
J. Waser
- 16:00 **Fluorinated Acyl Anhydrides in Switchable Divergent Photoredox Catalysis [OC-027]**
Rahul Giri, University of Fribourg
D. Katayev

Physical Chemistry [PC]

Session Endowment: Climeworks

Chairs: Prof. Cornelia Palivan, University of Basel
Prof. Thomas Bürgi, University of Geneva

- 10:45 **UV photoelectron spectroscopy of aqueous solutions [PC-011]**
Helen H. Fielding, University College London, UK
- 11:15 **Conformationally-selected ions for reactions with conformationally-selected molecules [PC-013]**
Jutta Toscano, University of Basel
L. Xu, S. Willitsch
- 11:30 **Low-frequency anharmonic couplings in bromoform revealed from 2D Raman-THz spectroscopy: From the liquid to the crystalline phase [PC-014]**
Seyyed Mousavi, University of Zurich
A. Berger, A. Shalit, P. Hamm
- 11:45 **Chiral control of spin-crossover dynamics in Fe(II) complexes [PC-015]**
Malte Oppermann, EPFL Lausanne
F. Zinna, J. Lacour, M. Chergui
- 12:00 **Source suppression and spin dynamics in hyperpolarized liquid state NMR spectroscopy by optically polarized crystals [PC-016]**
Federico De Biasi, EPFL Lausanne
P. Moutzouri, A. J. Parker, J. W. Blanchard, T. R. Eichhorn, I. Schwartz, L. Emsley
- 12:15 **Paramagnetic Properties of Neutral Sodium Doped Solvent Clusters [PC-017]**
Dominique Borgeaud, ETH Zurich
J. V. Barnes, E. Simmen, H. Yang, B. L. Yoder, R. Signorell
-
- 14:30 **Climeworks – from ETH start up to the world's leading direct air capture company [PC-021]**
Cornelius Gropp, Climeworks, Zurich
N. Casas, A. Vargas
- 15:00 **Solid-State Synthesis of cyclo Leu-Leu: The role of Packing [PC-023]**
Ariel Perez Mellor, University of Geneva
X. Wang, D. Rosa Gastaldo, C. Besnard, N. Giamboni, J. Brazard, T. Adachi, T. Buergi, A. F. Perez Mellor
- 15:15 **The travels of hydrogen over the catalyst surface [PC-024]**
Arik Beck, ETH Zurich
L. Artiglia, A. Kleibert, H. Frey, J. A. van Bokhoven
- 15:30 **Flash heating water through no man's land – Structural evolution and crystallization kinetics [PC-025]**
Constantin Krüger, EPFL Lausanne
G. Bongiovanni, N. J. Mowry, M. Drabbels, U. J. Lorenz
- 15:45 **EPR investigation of metal oxide catalysts: ferromagnetic behaviour induced by oxygen vacancies [PC-026]**
Mikhail Agrachev, ETH Zurich
T. Pinheiro Araújo, C. Mondelli, T. Zou, K. M. Engel, R. N. Grass, W. J. Stark, O. V. Safonova, S. Mitchell, J. Pérez-Ramírez, G. Jeschke
- 16:00 **At the Cutting Edge – NMR Studies Reveal Distinct Reactivities of Specific Edge Sites on Needle-Shaped γ -Al₂O₃ Nanocrystals Toward Pt(II) Precursors [PC-027]**
Laura Völker, ETH Zurich
J. Meyet, L. Rochlitz, C. Copéret

Polymers, Colloids & Interfaces [PI]

Session Endowment: BASF



Chairs: Dr. Dorina Opris, Empa Dübendorf
Dr. Dominik Brühwiler, ZHAW Wädenswil

- 10:45 **Leak-tight anastomosis hydrogel sealants using mutually interpenetrating networks [PI-011]**
Alexandre Anthis, ETH Zurich
- 11:15 **Recycling of waste polypropylene into high-value liquid hydrocarbons [PI-013]**
Shibashish Jaydev, ETH Zurich
A. J. Martín, M. Usteri, J. Pérez-Ramírez
- 11:30 **Colloidal synthesis of size and composition controlled alloy nanocrystals as selective alkyne semihydrogenation catalysts [PI-014]**
Jasper Clarysse, ETH Zurich
J. D. Silva, S. Zhang, S. Docherty, M. Yarema, C. Copéret, V. Wood
- 11:45 **Increasing the coverage of photoactive ligands on the surface of nanocrystals through a hybrid metal-oxide-ligand shell [PI-015]**
Philippe Green, EPFL Valais
O. Segura Lecina, P. P. Albertini, A. Loiudice, R. Buonsanti
- 12:00 **Self-assembly of lead halide perovskite nanocubes into multicomponent nanocrystal superlattices [PI-016]**
Ihor Cherniukh, ETH Zurich
T. V. Sekh, G. Rainò, T. Stöferle, M. Burian, A. Travasset, R. Erni, M. I. Bodnarchuk, M. V. Kovalenko
- 12:15 **Order and disorder in inverse Opals [PI-017]**
Jansie Smart, University of Fribourg
K. Dorbic, A. Parisotto, M. Lattuada
-
- 14:30 **Creating chemistry for a sustainable future in a world of change [PI-021]**
Olivier Enger, BASF Schweiz AG
- 15:00 **Transformer-Induced Metamorphosis of Polymeric Nanoparticle Shape at Room Temperature [PI-023]**
Kostas Parkatzidis, ETH Zurich
A. Anastasaki
- 15:15 **Mechanically morphing polymer systems [PI-024]**
Livius Muff, Adolphe Merkle Institute, University of Fribourg
C. Weder
- 15:30 **Interfacial rheology of particles with matching convex and concave asperities [PI-025]**
Lukas Woolley, ETH Zurich
F. Müller, D. Renggli, J. Vermant
- 15:45 **Lipidic based-gel with tunable release properties as a platform for local delivery of biotherapeutics [PI-026]**
Simone Aleandri, University of Bern
O. Elzenaty, P. Luciani
- 16:00 **Clusters of Hard-Soft Assembly for Bio-Applications [PI-027]**
Voichita Mihali, University of Basel
M. Skowicki, C. G. Palivan

POSTER SESSIONS**Poster Presentation Title [Code]**

First line = Presenting Author, Affiliation

Second line = Co-authors

**Analytical Sciences [AS]
Poster Session****Impact of Ablation Cell Design in LA-ICP-MS on Elemental Fractionation [AS-101]**

Pascal Becker, ETH Zurich

J. Koch, D. Günther

Harnessing low-temperature plasma chemistry to distinguish alkylated aromatic isomers with mass spectrometry [AS-102]

Alina Begley, ETH Zurich

R. Zenobi

Probing the Stability of the β -Hairpin Structure of GB1P in the Gas Phase by Coupling Mass Spectrometry and Fluorescence Spectroscopy [AS-103]

Lukas Benzenberg, ETH Zurich

A. S. Albrerini, R. W., J. B. Metternich, R. Zenobi

In-Cell Quantification of Drugs by Magic-Angle Spinning Dynamic Nuclear Polarization NMR [AS-104]

Pierrick Berruyer, EPFL Lausanne

A. Bertarello, M. Artelsmair, C. Elmore, S. Heydarkhan-Hagvall, M. Schade, E. Chiarparin, S. Schantz, L. Emsley

Visualizing Zeolite ZSM-5 Catalyst Deactivation at the Micro- and Nano-scales using Confocal and Tip-enhanced Fluorescence Microscopies [AS-105]

Siiri Bienz, ETH Zurich

N. Kumar, R. Zenobi

Novel Analytical Strategies for the Characterization of Peptide Complexes by Temperature-Controlled Cyclic Ion Mobility Mass Spectrometry [AS-106]

Philipp Bittner, ETH Zurich

V. Islami, T. Fiala, H. Wennemers, R. Zenobi

Solvent vapor removal for the downward-pointing ICP-TOFMS by using combined desolvation devices [AS-107]

Sandro Fazzolari, ETH Zurich

G. Niu, D. Günther

A new approach for determining RNA G-quadruplexes structures [AS-108]

Carla Ferreira Rodrigues, University of Zurich

Z. Wang, S. Jurt, S. Johannsen, R. K. Sigel

Development of a targeted proteomics method to monitor phosphorylation dynamics of multiple proteins within the mTOR pathway in zebrafish [AS-109]

Nikolai Huwa, EAWAG

R. Schönenberger, K. Groh

R-based Automatic Spectra Evaluation Routine (RASER) for the selective and rapid analysis of chlorinated paraffins and olefins [AS-110]

Marco Knobloch, Empa

O. Mendo Diaz, U. Stalder, F. Mathis, J. Hutter, S. Kern, L. Bigler, D. Bleiner, N. V. Heeb

Development of an Automated Total Nitrosamines (TONO) Analyzer [AS-112]

Minju Lee, EPFL Lausanne
W. Lee, Y. Lee, F. Breider, U. von Gunten

Time-resolved continuous measurements of DNA disposition kinetics using charged nanoparticles anchored on the ion-selective membrane of an aptamer-based electrode [AS-113]

Gabriel Mattos, University of Geneva
E. Bakker

Capacitive Readout of pH-Sensitive Membranes using a Symmetric Flow Cell towards Environmental Applications [AS-114]

Robin Nussbaum, University of Geneva
P. Kraikaew, S. Jeanneret, T. Cherubini, E. Bakker

Exploring Gas-Phase MS Methodologies for Structural Elucidation of Branched N-Glycan Isomers [AS-115]

Irina Oganessian, ETH Zurich

Effect of inert environment on Tip-Enhanced Raman Spectroscopy of biological molecules [AS-116]

Yashashwa Pandey, ETH Zurich
N. Kumar, R. Zenobi

XUV Desorption of Polymer Matrices studied with TOF-SIMS and XPS [AS-117]

Di Qu, University of Zurich
D. Bleiner, M. Wang, J. Wang, C. Masucci, D. Bleiner

Observation of calcium carbonate prenucleation species via dissolution dynamic nuclear polarization. [AS-118]

Yu Rao, EPFL Lausanne
M. Balodis, G. Stevanato, L. Emsley

A Comprehensive Method to Elucidate Pyoverdines Produced by Fluorescent Pseudomonas ssp. by UHPLC-HR-MS/MS [AS-119]

Karoline Rehm, University of Zurich
V. Vollenweider, R. Kümmerli, L. Bigler

Pressure drops set-up: an efficient way to rapidly measure the pressure drops contribution of novel catalysts. [AS-120]

Annalisa Sacchetti, Casale SA
M. Guiotto, J. D'Alessandri, P. Biasi

Portable and efficient suitcase for water measurements in Syngas and Ammonia Plants. [AS-121]

Annalisa Sacchetti, Casale SA
M. Guiotto, J. D'Alessandri, P. Biasi

Urea: from the laboratory to the plant scale to sustain the world's growth. [AS-122]

Annalisa Sacchetti, Casale SA
M. Canossi, C. Pizzolitto, A. Benedetti, L. Marrone, P. Biasi

Photoluminescence brightening of single-walled carbon nanotubes through conjugation with graphene quantum dots [AS-123]

Sayed Sajjadi, EPFL Lausanne
S. Wu, M. Reggente, N. Sharif, A. A. Boghossian

Simple micropreparative gel electrophoresis technique for purification of nanoscale materials [AS-124]

Sayed Sajjadi, EPFL Lausanne
S. Wu, V. Zubkovs, E. K. Goharshadi, H. Ahmadzadeh, A. A. Boghossian

Self-referencing Pulstrade: Further Optimization and New Electrode Designs [AS-125]

Ayian Speck, University of Geneva
E. Zdrachek, . Forrest, D. Migliorelli, S. Generelli, E. Bakker

Selective copper binding for accurate distance determinations by gas-phase transition metal FRET [AS-126]

Despoina Svingou, ETH Zurich
J. B. Metternich, R. Zenobi

Solvatochromic Co-extraction-based Optical Nanosensors for Monitoring Carbonate Speciation [AS-127]

Nikolai Tuftiakov, University of Geneva
K. J. Robinson, E. Bakker

New multiple nuclei and ultra-high resolution Spinsolve benchtop NMRs for 1- and 2D NMR assisted structure verifications [AS-128]

Harald Todt, Magritek GmbH

Robustness of the pure isotropic proton solid state NMR method [AS-129]

Daria Torodii, EPFL Lausanne
P. Moutzouri, B. Simões de Almeida, L. Emsley

Hydrogel matrices for near-infrared monitoring of ascorbic acid release [AS-130]

Hanxuan Wang, EPFL Lausanne
S. Çikrikci, X. Liu, A. A. Boghossian

Combining ion mobility spectrometry and fluorescence spectroscopy for structural characterization of biomolecules in the gas phase [AS-131]

Ri Wu, ETH Zurich
A. S. Albertini, R. Zenobi, S. Riniker

Self-powered potentiometric-optical transduction with capacitive electronic components [AS-132]

Yaotian Wu, University of Geneva
E. Bakker

Calibration Gas Generator for Secondary Electrospray Ionization High-Resolution Mass Spectrometry [AS-133]

Cedric Wüthrich, ETH Zurich
Z. Fan, G. Vergères, R. Zenobi, S. Giannoukos

Laser ablation mass spectrometry for imaging with improved sensitivity and throughput [AS-134]

Zuqiang Xu, ETH Zurich
D. Günther, B. Hattendorf

Catalysis Sciences & Engineering [CE] Poster Session**Structure of selective and non-selective dicopper (II) sites in CuMFI for methane oxidation to methanol [CE-101]**

Mikalai Artsiusheuski, ETHZ
J. A. van Bokhoven, V. Sushkevich

Insights into Lewis acidic nature of extra-framework aluminum centers incorporated in zeolites by ion-exchange [CE-102]

Syeda Batool, ETH Zurich
S. Vitaly, J. A. Bokhoven

Air and Moisture Tolerant Hydroamination Reactions using Alkali-Metal Amides as Catalysts [CE-103]

Sophia Belrhomari, University of Bern
L. J. Bole, E. Hevia

Identifying and Advancing Strategies for High-Yield Methane Partial Oxidation [CE-104]

Andrea Blankenship, ETH Zurich
Y. Ji, M. Ravi, M. Artsiusheuski, V. Sushkevich, J. A. van Bokhoven

Identification and Characterization of Active Sites in Copper Exchanged Mordenite in Direct Methane to Methanol Oxidation [CE-105]

Andreas Brenig, Paul Scherrer Institut, Villigen, ETH Zurich
J. W. Fischer, D. Klose, J. A. van Bokhoven, G. Jeschke, V. L. Sushkevich

Electrochemical Ruthenium-Catalysed C-H Activation in Water Through Heterogenization of a Molecular Catalyst [CE-106]

Jan Bühler, University of Zurich
J. Zurflüh, S. Siol, O. Blacque, L. Sévery, S. D. Tilley

Operando insight of polycrystalline nickel in ethylene to syngas self-sustained oscillatory conversion [CE-107]

Claudiu Colbea, ETH Zurich
M. Plodinec, L. Artiglia, J. A. van Bokhoven, M. Willinger

Bimetallic Gold-Zinc Catalysts for the Hydrogenation of CO₂ to Methanol [CE-108]

Scott Docherty, ETH Zurich
O. V. Safonova, C. Copéret

Production of Jet-Fuel-Range Olefins via Catalytic Conversion of Pentene and Hexene over Mesoporous Al-SBA-15 Catalyst [CE-109]

Florent Dubray, Paul Scherrer Institut, Villigen (Paul Scherrer Institut, Villigen)
V. Paunović, M. Ranocchiari, J. van Bokhoven

Automated image analysis for single-atom detection in catalytic materials by transmission electron microscopy [CE-110]

Dario Faust Akl, ETH Zurich
S. Mitchell, S. M. Collins, D. Garcia-Gasulla, J. Pérez-Ramírez

Reducing N₂O and NO_x emissions in Nitric acid plant with industrial Fe-zeolite catalysts [CE-111]

Alberto Garbujo, Casale SA
R. Lanza, E. Rohart, A. Lahougue, P. Biasi

Systematic investigation of the interaction between selected linear olefins and Zn-MOF-74 [CE-112]

Patrick Gäumann, Paul Scherrer Institut, Villigen
P. A. Rzepka, T. Fovanna, D. Ferrie, J. A. van Bokhoven, M. Ranocchiari

Promoted higher alcohols synthesis from syngas by inverse CuCo@ZrO₂ catalysts [CE-113]

Yuzhen Ge, ETH Zurich
J. Pérez-Ramírez

Unveiling evolution of active oxygen species in ethylene epoxidation over silver foil by ambient pressure X-ray photoelectron spectroscopy [CE-114]

Man Guo, ETH Zurich/Paul Scherrer Institut, Villigen
J. A. Bokhoven, L. Artiglia

⁵¹V ssNMR Study for Surface Site of Vanadium-based Olefin Polymerization Catalyst Supported on MgCl₂ [CE-115]

Yuya Kakiuchi, ETH Zurich
S. Sabisch, A. Yakimov, C. Copéret

Cooperative PYE Complexes and their Application in Formic Acid Dehydrogenation [CE-116]

Pascal Knörr, University of Bern
M. Albrecht

Activation of atomically-dispersed platinum in Pt/CeO₂ for the Water-Gas Shift reaction [CE-117]

Xiansheng Li, ETH Zurich
J. A. van Bokhoven, L. Artiglia

The hydrocarbon pool nature in the methanol-to-olefins process: an operando FT-IR spectroscopy study [CE-118]

Luca Maggiulli, Paul Scherrer Institut, Villigen
D. Ferri, J. A. van Bokhoven

Polarized nickel enables long-chain products in CO₂ electroreduction [CE-119]

Antonio Martín, ETH Zurich
Y. Zhou, F. Dattila, S. Xi, N. Lopez, J. Pérez-Ramírez, B. Yeo

The challenging interplay of catalyst, sorbent, and reactor in the sorption-enhanced methanol synthesis from CO₂ [CE-120]

Emanuele Moiola, Hitachi Zosen Inova

Droplet-based microfluidic platform for understanding metal stabilization in the design of single-atom heterogeneous catalysts [CE-121]

Thomas Moragues, ETH Zurich
S. Mitchell, D. Faust Akl, J. Pérez-Ramírez, A. deMello

A low Si/Al ratio in faujasites controls the selectivity in the catalytic fast pyrolysis of guaiacol [CE-122]

Zeyou Pan, Paul Scherrer Institut, Villigen
A. Puente-Urbina, A. Bödi, J. van Bokhoven, P. Hemberger

Assessing metal promotion in In₂O₃-catalyzed CO₂ hydrogenation using flame spray pyrolysis as a standardized synthesis platform [CE-123]

Thaylan Pinheiro Araújo, ETH Zurich
J. Morales-Vidal, T. Zou, R. García-Muelas, P. O. Willi, K. M. Engel, O. V. Safonova, D. Faust Akl, R. N. Grass, N. López, J. Pérez-Ramírez

Kinetic model of ammonia synthesis under industrial operating conditions [CE-124]

Cristina Pizzolitto, Casale SA
M. Guiotto, A. Biasin, P. Biasi

Study of reactivity of NH₃ synthesis via molecular modelling [CE-125]

Cristina Pizzolitto, Casale SA
D. Polino, L. Bonati, P. Biasi, R. Eckert, S. Reitmeier, R. Schlögl, M. Parrinello

Pd single-atom heterogeneous catalyst on nitrogen doped carbon for sustainable Sonogashira cross-coupling [CE-126]

Dario Poier, ETH Zurich
D. F. Akl, S. C. D'Angelo, S. Mitchell, S. Mitchell, S. Mitchell, S. Mitchell, G. Guillén-Gosálbez, J. Pérez-Ramírez, R. Martí

Towards parallel testing of CO₂ electroreduction to long-chain products [CE-127]

Phil Preikschas, ETH Zurich
A. J. Martín, J. Pérez-Ramírez

Insights into the Molecular Mechanism of Cobalt(II) Catalyzed C-O cross-Coupling Reaction: A DFT study [CE-128]

Chandralekha Rajalakshimi, Mahatma Gandhi University, Kottayam
A. Radhakrishnan, V. I. Thomas

Locating aluminum in zeolite frameworks by exploiting anomalous X-ray powder diffraction at the Al absorption edge [CE-129]

Przemyslaw Rzepka, ETH Zurich
A. B. Pinar, A. J. Knorpp, L. B. McCusker, C. Baerlocher, T. Huthwelker, J. A. van Bokhoven

Tin dendrite electrocatalyst for CO₂ reduction to formate over a broad potential window in a hybrid flow cell [CE-130]

Amrita Singh-Morgan, ETH Zurich
V. Mougél

Mechanistic Investigations of the Iron-Catalyzed Synthesis of Pyrrolidines by Intramolecular C-H Amination [CE-131]

Wowa Stroek, University of Bern
M. Albrecht

Ceria-supported gold nanoparticles as a superior catalyst for nitrous oxide production via ammonia oxidation [CE-132]

Ivan Surin, ETH Zurich
Z. Tang, A. Rasmussen, F. Krumeich, V. A. Kondratenko, J. Pérez-Ramírez

Sinter resistant nickel catalyst for lignin hydrogenolysis achieved by liquid phase atomic layer deposition of alumina [CE-133]

Farzaneh Talebkeikhah, EPFL Lausanne
S. Sun, W. Lan, J. Luterbacher

Effect of particle size in dibromomethane hydrodebromination over SiO₂-supported Pd nanoparticles [CE-134]

Matteo Vanni, ETH Zurich
V. Giulimondi, F. Krumeich, S. Mitchell, J. Pérez Ramírez

Unravelling the effect of bimetallic co-catalyst and reaction conditions on the photocatalytic conversion of methane to oxygenates over TiO₂ [CE-135]

Anna Wach, Paul Scherrer Institut, Villigen
D. Wierzbicki, M. Nachtegaal

Electrocatalytic generation of metal hydrides promoted by concerted proton electron transfer mediators [CE-136]

Alessandro Walker, ETH Zurich
V. Mougél

Pd/ZSM-5 materials for continuous liquid phase catalyzed methane oxidation to oxygenates [CE-137]

Dominik Wierzbicki, Paul Scherrer Institut, Villigen
A. Wach, D. Ferri, M. Nachtegaal

A Bioinspired Mo-based Electrocatalyst for efficient electrochemical nitrate reduction to ammonia [CE-138]

Yuan-Zi Xu, ETH Zurich
D. Abbott, V. Mougél

Boosting the formation of ethanol from CO₂ hydrogenation over Rh-based catalysts generated via SOMC [CE-139]

Wei Zhou, Zurich
C. Copéret

SOMC-Derived Cobalt Nanoparticles as Model for Conventional Heterogeneous Catalysts in CO_x Hydrogenation [CE-140]

Xiaoyu Zhou, ETH Zurich
G. Price, C. Copéret, G. Sunley

Revisiting Structure-Performance Relationships of Ni-Ga/SiO₂ Catalysts for the Hydrogenation of CO₂ to Methanol [CE-141]

Nora Zimmerli, ETH Zurich
P. M. Abdala, P. M. Abdala, C. R. Müller

Highly selective and stable ZnZrO_x catalysts prepared by flame spray pyrolysis for CO₂ hydrogenation to methanol [CE-142]

Tangsheng Zou, ETH Zurich
T. Pinheiro Araújo, J. Morales-Vidal, S. Verstraeten, P. O. Willi, M. Agrachev, G. Jeschke, N. López, J. Pérez-Ramírez

Computational and Theoretical Chemistry [CC] Poster Session**Solvation Free Energies in Subsystem Density Functional Theory [CC-101]**

Moritz Bensberg, ETH Zurich
P. L. Türtcher, J. P. Unsleber, M. Reiher, J. Neugebauer

Regression Transformer: Concurrent sequence regression and generation for molecular language modeling [CC-102]

Jannis Born, IBM Research Europe
M. Manica

Rationalizing Stereoselective Membrane Permeability of Mutanobactin D and Synthetic Analogues with Molecular Dynamic Simulations [CC-103]

Patricia Brandl, ETH Zurich
A. Albertini, S. Linker, F. Pultar, S. Riniker

Molecular Framework Analysis of the Drug-like Chemical Space [CC-104]

Ye Buehler, University of Bern
J. L. Reymond

Efficient linear-response TDDFT implementation for core-level spectroscopy of large and periodic systems [CC-105]

Augustin Bussy, University of Zurich

Accessing the complex free energy landscape of any (photoswitchable) organocatalysts with a quantum chemical accuracy [CC-106]

Frederic Celerse, EPFL Lausanne
R. Fabregat, S. Vela, S. Gallarati, C. Corminboeuf

Predicting Multiple Ligand Binding Affinities from Single Alchemical Free Energy Calculations [CC-107]

Candide Champion, ETH Zurich
R. Gall, B. Ries, S. Rieder, E. P. Barros, S. Riniker

PGT: A machine learning model to accelerate IP generation in chemistry [CC-108]

Dimitrios Christofidellis, IBM Research

Chemical shift-dependent interaction maps in molecular solids [CC-109]

Manuel Cordova, EPFL Lausanne
L. Emsley

Implementation of Nuclear Velocity Perturbation and Magnetic Field Perturbation Theory in CP2K and Their Application to Vibrational Circular Dichroism [CC-110]

Edward Ditler, University of Zurich

On the quantum chemical roots of molecular similarity descriptors for machine learning [CC-111]

Stefan Gugler, ETH Zurich
M. Reiher

Automatic purpose-driven basis set truncation for time-dependent Hartree-Fock and time-dependent density-functional theory [CC-112]

Ruo Cheng Han, University of Zurich
J. Mattiat, S. Lubner

Scrutinizing Semi-empirical Methods for Excited Electronic States [CC-115]

Veronika Klasovita, ETH Zurich
T. Weymuth, M. Reiher

NaviCat: Computational Tools to Navigate Molecular Catalyst Landscape [CC-116]

Ruben Laplaza, EPFL Lausanne
M. D. Wodrich, S. Das, S. Gallarati, C. Corminboeuf

Quantifying Tunnelling in Molecules and Clusters with Instanton Theory [CC-117]

Gabriel Laude, ETH Zurich
J. O. Richardson

Nonadiabatic processes in condensed phase systems with Δ SCF [CC-119]

Momir Mališ, University of Zurich
E. Vandaele, S. Lubner

Quantum Effects in Photosensitization: Possibility of Tunneling? [CC-120]

Meghna Manae, ETH Zurich
J. O. Richardson

DFT-Based Mechanistic Investigation Of Zinc(II) Catalyzed O-Arylation Reaction [CC-121]

Lydia Mathews, Mahatma Gandhi University
C. Rajalakshmi, P. Santhoshkumar, V. I. Thomas

Spectroscopic simulations with real-time TDDFT - linear response and gauge dependence [CC-123]

Johann Mattiat, University of Zurich
S. Lubner

The variational Gaussian approximation combined with high-order geometric integrators with applications to quantum tunneling and vibronic spectra [CC-124]

Roya Moghaddasi Fereidani, EPFL Lausanne
J. Vanicek

Streamlined Automatic Active Space Calculations through AutoCAS [CC-125]

Maximilian Mörchen, ETH Zurich
C. J. Stein, M. Reiher

Bachelor Students' Understanding of Basic Quantum Chemical Concepts [CC-126]

Charlotte Müller, ETH Zurich
M. Kapur, M. Reiher

Bayesian Optimisation-accelerated Additives Screening and Yield Improvements in Chemical Reactions [CC-127]

Bojana Ranković, EPFL Lausanne
R. Griffiths, H. Moss, P. Schwaller

A Density Functional Theory Investigation on the Mechanism of Ligand-Free Manganese Catalyzed Ullmann Reaction [CC-128]

Parvathi Santhoshkumar, Mahatma Gandhi University
R. Sulay, V. I. Thomas

Deep learning assisted Suzuki cross coupling catalyst design [CC-130]

Oliver Schilter, EPFL Lausanne & IBM Research Europe
A. Vaucher, T. Laino

Novel approaches for chiral spectroscopy of periodic systems [CC-131]

Lukas Schreder, University of Zurich
S. Lubner

Excited-State Properties for Extended Systems: Efficient Hybrid Density Functional Methods [CC-132]

Beliz Sertcan, University of Zurich
A. Hehn, F. Belleflamme, S. Chulkov, M. Watkins, J. Hutter

Double-hybrid density functionals for the condensed phase: Gradients, stress tensor, and auxiliary-density matrix method acceleration [CC-133]

Frederick Stein, University of Zurich

Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis [CC-134]

Miguel Steiner, ETH Zurich
M. Reiher

Computational Study on Multicopper Oxidase-mediated Biotransformations [CC-135]

Vincenz-Maria Steiner, University of Zurich
H. Satoh, J. Hutter, K. Fenner, A. Athanasakoglou, J. Hutter

Computational Design of Capping Ligands for Lead Halide Perovskite Nanocrystals [CC-136]

Andriy Stelmakh, ETH Zurich
V. Morad, M. Svyrydenko, L. Feld, M. Aebli, A. Baumketner, M. V. Kovalenko

A generalized machine learning framework to predict the space-time yield of thermocatalytic CO₂ hydrogenation to methanol [CC-137]

Manu Suvarna, ETH Zurich
T. Pinheiro Araújo, J. Pérez-Ramírez

The chemistry puppeteer: enhancing the diversity of single-step retrosynthesis [CC-138]

Alessandra Toniato, IBM Research Europe
A. C. Vaucher, P. Schwaller, T. Laino

Chemoton: Automated Exploration of Reaction Networks [CC-139]

Jan Unsleber, ETH Zurich
S. A. Grimmel, M. Reiher

The Transferability Limits of Static Benchmarks [CC-140]

Thomas Weymuth, ETH Zurich
M. Reiher

Capturing tunnelling and wavepacket splitting effects on electronic spectra with Hagedorn wavepackets [CC-141]

Zhan Tong Zhang, EPFL Lausanne
J. Vaníček

Generalizing Collective Variables using Deep Learning for Free Energy Surface Calculation [CC-142]

Rangsiman Ketkaew, University of Zurich
F. Creazzo, S. Luber

Chemistry and the Environment [EV] Poster Session

Significant Enhancement in Performance of Sb_2Se_3 Photocathode via Sequential Etching and $CuCl_2$ Treatment [EV-101]

Pardis Adams, University of Zurich

Biodegradation of mulch films in Swiss agricultural soils assessed in laboratory, mesocosm and field incubations [EV-102]

Silvan Arn, ETH Zurich

The Bioaccumulation of Anionic and Cationic Organic Compounds in Rainbow Trout Cell [EV-103]

Fabian Balk, Eawag Dübendorf
B. Hüssler, J. Hollender, K. Schirmer

Solution and gel-phase quantification of lignin structural features with improved 2D-HSQC₀ NMR processes [EV-104]

Claire Bourmaud, EPFL Lausanne
S. Bertella, J. S. Luterbacher

Efficacy of environmental friendly iron-based metal-organic framework/polymer composites to reduce silver ion toxicity to Zebrafish embryos (*Danio rerio*) [EV-105]

Veysel Demir, Eawag

Non-target screening reveals the identity of carbonous and nitrogenous carbonyl-containing oxidation byproducts formed during ozonation of various water types [EV-107]

Joanna Houska, Eawag
T. Manasfi, I. Gebhardt, U. von Gunten

Biotransformation capacity for trace contaminants - from wastewater to natural surface water [EV-108]

Martina Kalt, Eawag / University of Zurich
E. Ceppi, Y. Yu

Insights on the carbonation mechanism of alkali metal nitrate promoted MgO by ¹⁸O isotope labeling [EV-109]

Annelies Landuyt, ETH Zurich
P. V. Kumar, P. M. Abdala, A. H. Bork, C. R. Müller

The Impact of Temperature on Biodegradation of Poly-3-hydroxybutyrate-3-hexanoate (PHBH) in Soil [EV-110]

Juliana Laszakovits, ETH Zurich
R. Kaegi, M. Sander, K. McNeill

Development of an Automated Total Nitrosamines (TONO) Analyzer [EV-111]

Minju Lee, EPFL Lausanne
W. Lee, Y. Lee, F. Breider, U. von Gunten

Antibiotic uptake by spinach (*Spinacia oleracea*) and radish (*Raphanus sativus*) - distribution between above- and belowground plant fractions, soil, and soil pore-water [EV-112]

Inna Nybom, ETH Zurich
S. van den Broek, T. D. Bucheli, C. S. McArdell, G. Garland

Mineralizing Wood using Clock Reactions [EV-113]

Guido Panzarasa, ETH Zurich
R. Kürsteiner, I. Burgert, G. Panzarasa

Bioinspired Polymetallic Sulfido Clusters for Nitrate and Nitrite Reduction to Ammonia [EV-114]

Marie Perrin, ETH Zurich
V. Mougél

Bio-oil Deoxygenation: A Contribution Towards a Sustainable Society [EV-115]

Stephan Pollitt, Paul Scherrer Institut, Villigen
C. Ehinger, O. Sofanova, M. Nachtegaal, C. Copéret

Characterization of reactive nitrogen moieties in natural organic matter with different methodologies: oxidative and stable isotopic approach [EV-116]

Jiwoon Ra, Eawag
U. von Gunten

Simulation of Realistic Aqueous Ozonation Conditions: Use of Small Scavenger Molecules as Surrogate for Dissolved Organic Matter [EV-117]

Simon Rath, Eawag
U. von Gunten

Speed it up: How temperature drives toxicokinetic processes in aquatic invertebrates [EV-118]

Johannes Raths, Eawag
J. Hollender

Ferrate (VI) oxidation of primary amines in water: kinetics, reaction products and implication for N-containing byproduct formation [EV-119]

Valentin Rougé, Eawag
P. Nguyen, S. Allard, Y. Lee

Porous Polyisothiocyanurates for Selective Palladium Recovery and Heterogeneous Catalysis [EV-120]

KyungSeob Song, University of Fribourg
T. Ashirov, S. Naidu Talapaneni, A. Hugh Clark, A. Yakimov, M. Nachtegaal, C. Copéret, A. Coskun

Heavy metals in agricultural urban and semi-urban soils and vegetables in Havana, Cuba. [EV-121]

Dayana Sosa, Centro Nacional de Sanidad Agropecuaria (CENSA)
D. Buerge-Weirich, I. Hilber, R. Faure, T. Bucheli, A. Escobar

First steps toward sustainable circular uses of chemicals: advancing the assessment and management paradigm [EV-122]

Zhanyun Wang, EMPA
S. Hellweg

Permanganate reduction by hydrogen peroxide: formation of reactive manganese species and superoxide and enhanced micropollutant abatement [EV-123]

Ke Xu, Eawag, Dübendorf
U. von Gunten, U. von Gunten

Assessment of chlorine stability in recycled handwashing water: Role of amide-type compounds from soaps [EV-124]

Tianqi Zhang, EPFL Lausanne
U. von Gunten

**Inorganic Chemistry [IC]
Poster Session**
Watching Ternary Oxides with Dual Eyes: an *in-situ* Two-Colour XES Studies of Photo-Electrocatalytic Water Oxidation Mechanisms in Ferric Pseudobrookite (Re₂TiO₅) Photoanodes [IC-101]

Devi Prasad Adiyeri Saseendran, University of Zurich
S. Peredkov, C. Triana, D. Abbott, V. Mougel, G. R. Patzke, S. DeBeer

Developing the biological potential of organometallic cages [IC-102]

Santiago Luis Alles, University of Neuchâtel
B. Therrien

Redox Chemistry of Corrin-Based F430 Mimics [IC-103]

Samira Amini, University of Zurich
C. Brenig, F. H. Zelder

Series of low-valent uranium-based coordination polymers based on tritopic carboxylic acids [IC-104]

Andrei Andreichenko, EPFL Lausanne
A. Willauer, F. Fadaei-Tirani, R. Scopelliti, A. Chauvin, M. Mazzanti

Controlled Modification of Cobalt Phosphide Catalysts by Sulfur [IC-105]

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

Quantum crystallographic evaluation of S-C and P-C bonds in sulfur and phosphorus ylides [IC-106]

Yaser Balmohammadi, University of Bern
S. Grabowsky, L. Malaspina

Structure and characterisation of a series of bipyrimidine-bridged diuranium complexes [IC-107]

Mikhail Batov, EPFL Lausanne
D. K. Modder, T. Rajeshkumar, A. Sienkiewicz, A. Sienkiewicz, I. Živkovič, R. Scopelliti, L. Maron, M. Mazzanti

Selective Olefin Transfer Hydrogenation of Unsaturated Carbonyls with EtOH using a PYA-based Ruthenium (II) Complex [IC-108]

Alicia Beaufils, Universität Bern
M. Albrecht

⁹⁹Tc-PNP Pincer Complexes interacting with Small Molecules [IC-109]

Manuel Besmer, University of Zurich
H. Braband, R. Alberto

Environmental Pollutant Gas Sensing Inspired by Polyoxometalate-Mediated Aerobic Oxidation Catalysis [IC-110]

Máté Bezdek, ETH Zurich
T. M. Swager

Strongly confined CsPbBr₃ perovskite quantum dots as quantum emitters and building blocks for highly ordered rhombic superlattices [IC-111]

Simon Boehme, ETH Zurich
M. I. Bodnarchuk, M. Burian, F. Bertolotti, I. Cherniukh, N. Masciocchi, S. D. Stranks, G. Rainò, A. Guagliardi, M. V. Kovalenko

Synthesis, Structure and Bonding of Alkali-Metal Nickelates [IC-112]

Andryj Borys, University of Bern
E. Hevia

An Orthogonal Labeling Strategy to Accelerate Bioconjugation of [^{99m}Tc]-Building Blocks [IC-113]

Henrik Braband, University of Zurich
M. Schnierle, M. Ringenberg, R. Alberto

Investigation of Different Deposition Techniques of Holmium Sources for the Measurement the Electron Neutrino Mass [IC-114]

Noemi Carboni, Paul Scherrer Institut, Villigen
G. L. de Bodin de Galembert, P. J. Steinegger, E. A. Mauger

Electric Field Effects on the Surface Chemistry of Inorganic Materials [IC-115]

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

Structure-function correlations in a new family of homoleptic tris-didentate Cr(III) complexes. [IC-116]

Julien Chong, University of Geneva
A. Benchohra, C. M. Cruz, C. Besnard, L. Guenée, C. Piguet

Diimine Re(I) tricarbonyl complexes: toward novel highly potent and non-toxic antimicrobial agents [IC-117]

Youri Cortat, University of Fribourg
S. Nasiri Sovari, N. Radakovic, F. Zobi, A. Pavic

Dioxygen Activation in Rieske Dioxygenases: A Model Study Towards Automated QM/MM Protocols [IC-118]

Katja Csizi, ETH Zurich
C. Brunken, L. Eckert, M. Reiher, T. B. Hofstetter

Tuning spin-crossover transition temperatures in non-symmetrical homoleptic meridional/faceal [Fe(didentate)₃]²⁺ complexes [IC-119]

Neel Deorukhkar, University of Geneva
L. Guénée, C. Piguet

Redesigning nanocrystal synthesis - Critically evaluating the use of solvents and ligands [IC-120]

Evert Dhaene, University of Basel
K. M. Jensen, P. F. Smet, K. De Buysser, I. Van Driessche, J. De Roo

Development of an electrochemical strategy for routine separations of radionuclides [IC-121]

Paul Dutheil, Paul Scherrer Institut, Villigen
D. Herrmann, P. Steinegger, M. Heule

Reversible fac-mer Isomerization of Luminescent Ir(III) Complexes [IC-122]

Anastasia Gitlina, EPFL Lausanne
K. Severin

¹⁰⁹Ag NMR Chemical Shift: A Descriptor of Brønsted Acidity from Molecular Ag-NHC-Complexes [IC-123]

Colin Hansen, ETH Zurich
S. R. Docherty, W. Cao, A. Yakimov, C. Copéret

Lanthanide Isotopes in Uranium Products [IC-124]

Michael Hofstetter, ETH Zurich
S. Röllin, J. Corcho Alvarado, P. Steinegger

Reactivity of Multimetallic Thorium Nitrides Generated by Reduction of Thorium Azides [IC-125]

Fang Hsueh, EPFL Lausanne
L. Barluzzi, M. Keener, T. Rajeshkumar, R. Scopelliti, L. Maron, M. Mazzanti

Potassium Alkoxide Mediated Zincations of Aromatic Substrates [IC-126]

Neil Judge, University of Bern
E. Hevia

From Macrocycles into Assembled Chain-mails! [IC-127]

Ali Kaiss, University of Fribourg
A. Hinaut, A. Crochet, E. Meyer, K. M. Fromm

Isocyanides and their Strong Affinity to Gold [IC-128]

Charlotte Kress, University of Basel
M. Mayor

Photoinduced Electron-Transfer Through the Mechanical Bond in a Supramolecular Dyad [IC-129]

Subhradip Kundu, University of Geneva
C. B. Larsen, C. B. Larsen

Bifunctionalised Vitamin B12 Derivatives for Medicinal Applications [IC-130]

Paula Mestizo, University of Zurich
C. Brenig, F. Zelder

The development of new luminescent MOFs for molecular detection. [IC-131]

Franck Oswald, University of Fribourg
A. Kastrati, J. Hankache, K. M. Fromm

Anti-Cancer Activity of Polyoxometalates and their Nanocomposites [IC-132]

Jaclyn Parris, University of Zurich
G. Wiprächtiger, R. Hooshmandabbasi, G. Patzke, C. Maake

The chemistry of Cu₃N and Cu₃PdN nanocrystals [IC-133]

Mahsa Parvizian, University of Basel
A. Duràn Balsa, R. Pokratath, C. Kalha, S. Lee, D. Van den Eynden, M. Ibáñez, A. Regoutz, J. De Roo

Mechanistic insights into multi-photon driven photocatalysis and its application for challenging redox catalysis [IC-134]

Björn Pfund, University of Basel
D. Schaad, O. S. Wenger

Mechanistic Insight into the Precursor Chemistry of ZrO₂ and HfO₂ Nanocrystals; towards Size-Tunable Syntheses [IC-135]

Rohan Pokratath, University of Basel
D. Van den Eynden, S. R. Cooper, J. K. Mathiesen, V. Waser, M. Devereux, S. Billinge, M. Meuwly, K. Jensen

Novel Re (I) tricarbonyl complexes of thiazolhidrazinylidene-chroman-2,4-diones [IC-136]

Fatinda Rahmani, University of Fribourg
F. Rahmani, A. Crochet, F. Zobi

Electronically flexible pyridyl-pyridylidene amide ligands for palladium-catalyzed α -arylation of ketones [IC-137]

Esaie Reusser, University of Bern
M. Albrecht

Demonstrating and unraveling a controlled nanometer-scale expansion of the vacancy defects in graphene by CO₂ [IC-138]

Mojtaba Rezaei, EPFL Lausanne
L. F. Villalobos, K. V. Agrawal

Novel manganese complexes with phenolate-substituted NHC ligands: catalytic application in the oxidation of organic compounds [IC-139]

Giacomo Rigoni, University of Bern
P. Nylund, M. Albrecht

Maturarbeit: Towards a copper-Azophloxine inorganic complex for the selective naked-eye detection of pyrophosphate in water [IC-140]

Thibaud Rossel, University of Neuchâtel
A. Bieri, T. Rossel

Initiation of Methyltrioxorhenium by C–H Activation in Homogeneous Olefin Metathesis Catalysts [IC-141]

Yannick Stöferle, ETH Zurich
P. Chen

Transactinide chemistry in the sub-second regime using vacuum adsorption chromatography [IC-142]

Georg Tiebel, ETH Zurich/ Paul Scherrer Institut, Villigen
R. Dressler, R. Eichler, P. Steinegger

Zirconium and hafnium metal oxo clusters as smallest conceivable nanocrystals; from synthesis to application [IC-143]

Dietger Van den Eynden, University of Basel

High Temperature Studies with 4H-SiC α -Detectors for Future Superheavy Element Experiments [IC-144]

Jennifer Wilson, Paul Scherrer Institut, Villigen/ETH Zurich
M. Camarda, M. Carulla, G. Tiebel, R. Dressler, P. Steinegger

Evaporation of polonium from heavy-liquid-metal-cooled reactors [IC-145]

Ivan Zivadinovic, ETH Zurich
L. Lu, P. J. Steinegger, J. Neuhausen

Dinuclear uranium nitride complexes for small molecule transformations [IC-146]

Megan Keener, EPFL Lausanne
M. Mazzanti, M. Keener

Medicinal Chemistry & Chemical Biology [MC] Poster Session**Site-specific labeling of large RNAs for single-molecule FRET [MC-101]**

Esra Ahunbay, University of Zurich
S. Zelger-Paulus, R. K. Sigel

From mixed-chirality to mixed peptide-peptoids antimicrobial peptides to control multidrug resistant Gram-negative bacteria [MC-102]

Etienne Bonvin, University of Bern
J. Reymond

Genome-wide mapping of *O*⁶-methylguanine [MC-103]

Jasmina Büchel, ETH Zurich
C. Mingard, P. Reinert, S. Huber, S. J. Sturla

Overcoming aggregation in the chemical synthesis of c-Myc[86-143] [MC-104]

Héloïse Bürgisser, University of Zurich
R. Lescure, B. Tamás, E. T. Williams, N. Hartrampf

Advanced NMR Methods Enable the Identification and Structure-Activity Relationship of K-Ras Ligands [MC-105]

Matthias Bütikofer, ETH Zurich
F. Torres, G. Stadler, H. Kadavath, J. Orts, R. Riek

Fluorescent labeling of cellular DNA for an exploration of in-situ chromatin structure [MC-106]

Wei Cai, EPFL Lausanne
M. Mivelaz, B. Fierz, B. Fierz

Stereorandomized Antimicrobial peptide dendrimers from Chemical Space against multidrug-resistant bacteria [MC-107]

Xingguang Cai, University of Bern
M. Orsi, A. Capecchi, S. Javor, J.-L. Reymond

Production of Semisynthetic Tubulin with Definable Post-Translational Modification [MC-108]

Po-Han Chang, EPFL Lausanne
E. Ebberink, S. Fernandes, C. Aumeier, B. Fierz

Fluorescent LLOs – Shedding light on OST and ALG enzymes [MC-109]

Mario de Capitani, University of Bern
J.-L. Reymond

Frame Shifts Affect the Stability of Collagen Triple Helices [MC-111]

Tomas Fiala, ETH Zurich
E. P. Barros, M. Ebert, E. Ruijsenaars, S. Riniker, H. Wennemers

Developing Molecular Tools for the Study and Detection of Calcium-Sensing Receptor (CaSR) in Parathyroid Glands [MC-112]

Jérôme Fischer, University of Bern
M. Lochner

Design and Biological evaluation of Drug-Like Inhibitors Targeting the Allosteric Site of the SARS-CoV-2 Main Protease Enzyme [MC-113]

Mohammad Ghattas, Al Ain University, Abu Dhabi
L. Alzyoud, F. Mohamed, B. R. Ali, W. Rabeh, N. Atatreh

Lanthanide-Functionalized Lithium Niobate Nanoparticles for Multimodal Imaging [MC-114]

Adrian Gheata, EPFL Lausanne
A. Spada, S. Dumolard, M. Wittwer, P. Llussa, L. Bonacina, A. Chauvin, S. Gerber-Lemaire

Rapid Synthesis of Trifunctionalised Chemical Biology Probe from Unprotected L-Cysteine [MC-115]

Philipp Grossenbacher, University of Bern
M. Lochner

Structure-based modelling of HIF2 α warheads for PROTAC design [MC-116]

Margaux Héritier, University of Geneva
C. Cecchini, V. Trush, F. L. Gervasio, F. Rastinejad, L., L. Scapozza

A Locally Activatable Sensor for Robust Quantification of Organellar GSH [MC-117]

Sarah Hübner, EPFL Lausanne
G. Quargnali, S. Thallmair, P. Rivera-Fuentes

New Fidaxomicin Antibiotics: Combining Metabolic Engineering and Semisynthesis [MC-118]

Erik Jung, University of Zurich
M. Hunter, J. Costafrolaz, Y. Mattenberger, S. Dittmann, D. Schäfle, T. Griesser, P. Sander, S. Sievers, R. Müller, K. Gademann

Stapled-Peptide PROTACs by Hypervalent Iodine Staples [MC-119]

Yuji Kamei, EPFL Lausanne

J. Waser, B. Fierz

Aryltetralin lignans from *Hyptis brachiata* inhibiting human T-cell proliferation [MC-120]

Morris Keller, University of Basel
M. Winker, N. Sperisen, M. Gupta, M. Hamburger, C. Gründemann, O. Poterat

A short motif goes a long way: How minimal ribozymes make large proteins redundant [MC-121]

Kasimir Kienbeck, University of Zurich
L. Malferttheiner, S. Zelger-Paulus, S. Johannsen, C. von Mering, R. K. Sigel

Engineering nonviral protein cages for delivery applications [MC-122]

Mikail Levasseur, ETH Zurich
D. Hilvert

Determining the redox state of the Golgi apparatus by using genetically encoded tools [MC-123]

Carla Miró-Vinyals, University of Zurich
S. Hübner, G. Grammbitter, P. Rivera-Fuentes

Purification-free synthesis and screening of thousands of cyclic peptides [MC-124]

Alexander Nielsen, EPFL Lausanne
A. S. Zarda, Z. Bognar, G. K. Mothukuri, C. Heinis

Synthesis and biological evaluation of small-molecule inhibitors of Tumor Necrosis Factor Receptor 1 (TNFR1) [MC-125]

Sara Pannilunghi, University of Geneva
S. Tardy, A. Gouiller, M. Héritier, D. Pejoski, L. Scapozza

X-ray Structures of Mixed-chirality α -Helical Antimicrobial Peptides [MC-126]

Hippolyte Personne, University of Bern
A. Stocker, S. Javor, J. L. Reymond

Photopharmacology and smart biocompatible materials based on cyclic dipeptides. [MC-127]

Zbigniew Pianowski, Karlsruhe Institute of Technology KIT
S. Kirchner, A. Leistner, P. Gödtel, A. Seliwjorstow, V. Schäfer, Z. L. Pianowski

Fluorescence-guided Quantification and Mapping of DNA Damage in the Human Genome [MC-128]

Nikolai Püllen, ETH Zurich
V. Takhaviev, N. K. Singh, A. Poetsch, H. Gahlon, S. J. Sturla

The sulfonated Molybdenum Cofactor influences the Structure of the moaA riboswitch [MC-129]

Maria Reichenbach, University of Zurich
F. Amadei, S. Gallo, R. K. Sigel

Nanopore detection of carboxymethylated DNA bases [MC-130]
Emma Sandell, ETH Zurich

Thiolation and Carboxylation of Glutathione Synergistically Enhance Its Lead-Detoxification Capabilities [MC-131]

Luca Sauser, Universität Zürich
T. A. Mohammed, L. Rulíšek, M. S. Shoshan

Homologous N-acyl ethanolamines from the *C. elegans* exometabolome [MC-132]

Marie-Désirée Scheidt, University of Neuchatel
S. Bandi, S. von Reuss

Turn-on Fluorescent Peptide Conjugates for the Detection of Human Monoamine Oxidase Enzymes [MC-133]

Adeline Schmitt, ETH Zurich
M. R. Aronoff, M. Li, H. Wennemers

BODIPY-Based Photothermal Agents for Cancer Treatment [MC-134]

Lukas Schneider, University of Zurich
M. Kalt, S. Koch, S. Sithamparamanathan, V. Villiger, J. Mattiat, F. Kradolfer, S. Luber, M. Bonmarin, B. Spingler

Impacts of DNA repair on anticancer drugs: synthesis and activity of novel acylfulvene analogs with aromatic groups [MC-135]

Laura Slappendel, ETH Zurich
C. M. Aloisi, O. D. Schärer, S. J. Sturla

Surface functionalization of harmonic nanoparticles with proteins for cancer active targeting [MC-136]

Alessandra Spada, EPFL Lausanne
A. Gheata, E. Ansart, M. Wittwer, S. Gerber-Lemaire

Facile Preparation of UFMylation Activity-Based Probes by Chemoselective Installation of Electrophiles at the C-terminus of Recombinant UFM1 [MC-137]

Kateryna Tolmachova, ETH Zurich
J. Farnung, J. Liang, J. E. Corn, J. W. Bode

Targeting RNA G-quadruplex to combat SARS-CoV-2 [MC-138]

Haibo Wang, University of Zurich

Flow chemical synthesis to study the regulatory role of post-translational modifications (PTMs) and PTM-crosstalk on c-Myc [MC-139]

Elyse Williams, University of Zurich
M. Schuster, O. Zerbe, N. Hartrampf

Stapled-Peptide PROTACs by Hypervalent Iodine Staples [MC-140]

Yuji Kamei, EPFL Lausanne
B. Fierz, J. Waser

Discovery and characterization of ACT-284069, a double prodrug of the P2Y₁₂ receptor antagonist selatogrel [MC-141]

Eva Caroff, Idorsia Pharmaceuticals Ltd
F. Hubler, C. Gnerre, A. Treiber

Organic Chemistry [OC] Poster Session

Benzylic Metalation of Toluenes Using a Hydrocarbon Soluble Sodium Alkyl Reagent [OC-101]

David Anderson, University of Bern
A. Tortajada, E. Hevia

Performance boost of a merocyanine photoacid by supramolecular encapsulation [OC-102]

Cesare Berton, EPFL Lausanne
C. Pezzato

The Bioorthogonal C₃N-Cyclic Azomethine Imine-Isonitrile Ligation [OC-103]

Maurice Biedermann, ETH Zurich
A. Markos, H. Wennemers

Tosyloxybenziodoxolone: a platform for the umpolung of alkynes [OC-104]

Julien Borrel, EPFL Lausanne
J. Waser

Organocatalyzed Conjugate Addition Reactions of Aldehydes to Nitroolefins with Anti-Selectivity [OC-105]

Alena Budinská, ETH Zurich
T. Schnitzer, H. Wennemers

Cyclopentadienone Iron Complex Catalyzed Hydrogenation of Ketones: An Operando Spectrometric Study Using Pressurized-Sample-Infusion Electrospray-Ionization Mass-Spectrometry [OC-106]

André Bütikofer, ETH Zurich
P. Chen

Accessing Asymmetric Nickel-Catalyzed Carbonyl α C-H bond Functionalization [OC-107]

Yixuan Cao, EPFL Lausanne
M. Wodrich, N. Cramer

Direct Photoexcitation of Ethynylbenziodoxolones: An Alternative to Photocatalysis for Alkynylation Reactions [OC-108]

Diana Cavalli, EPFL Lausanne
S. G. Amos, F. Le Vaillant, J. Waser

Thiol-Mediated Uptake and Inhibition of Phosphorothioate-Derived Transporters [OC-109]

Filipe Coelho, University of Geneva
Q. Laurent, N. Sakai, S. Matile

Geländer Molecules with orthogonal joints: Design and Synthesis of Macrocyclic Dimers [OC-110]

Adriano D'Addio, University of Basel
J. Malincik, O. Fuhr, D. Häussinger, M. Mayor

HTE/Data Science Augmented Investigation of NiZn Nanocrystal Catalyzed Alkyne Semihydrogenation [OC-111]

Jordan De Jesus Silva, ETH Zurich
J. Clarysse, S. Zhang, S. R. Docherty, M. Yarema, V. Wood, C. Copéret, V. Wood, C. Copéret

Flow Chemistry for the Chemo-Enzymatic Synthesis of Anaesthetics [OC-112]

Pablo Diaz-Kruik, University of Bern
D. Roura Padrosa, A. Benítez-Mateos, D. Lim, F. Paradisi

Arene-Limited Non-directed C–H Arylation of Fluoroarenes [OC-113]

Chao Dong, University of Zurich
M. Örgen, I. Čorić

Regioselective Synthesis of (Highly) Substituted Vinyl Ethers through a One-Pot Palladium-Catalyzed Assisted Tandem Olefin Migration/Heck Reaction [OC-114]

Thomas Duhamel, University of Geneva
C. Mazet

Regulation Through Contortion: From Supramolecular Surface-Interaction to Tunable Spin Information Relays [OC-115]

Mélissa El Bitar Nehme, University of Zurich
M. Rickhaus

New Cationic Helical Dyes through Late-Stage Functionalization and their Electronic and (Chir)Optical Properties [OC-116]

Bibiana Fabri, University of Geneva
L. Frédéric, F. Zinna, G. Pescitelli, T. Funaioli, L. Di Bari, J. Lacour

Towards Radial Polymers as an Alternative to SWNCTs [OC-117]

Sergey Fisher, University of Bern
T. Šolomek

Regio- and Enantioselective Copper-Catalyzed Protoboration of 1,1-Disubstituted Enecarbamates [OC-118]

Arthur Flaget, University of Geneva
C. Mazet

Pd(II)/(IV)-Redox Cycle Enabled Oxidative [2+2] Annulation between Aryl Boronic Acids and Olefins [OC-119]

Takuji Fujii, EPFL Lausanne
S. Gallarati, C. Corminboeuf, Q. Wang, J. Zhu

OSCAR: An Extensive Repository of Chemically and Functionally Diverse Organocatalysts [OC-120]

Simone Gallarati, EPFL Lausanne
P. E. van Gerwen, R. Laplaza, C. Corminboeuf

Shape-Assisted Self-Assembly of Carpyridines into 1D Stacks [OC-121]

Lucía Gallego, University of Zurich
J. Woods, A. Vargas Jentzsch, M. Rickhaus

Single-atom heterogeneous catalysts for sustainable organic synthesis [OC-122]

Georgios Giannakakis, ETH Zurich
S. Mitchell, J. Pérez-Ramírez

Multi-Photon Excitation with Red Light in Photoredox Catalysis [OC-123]

Felix Glaser, University of Basel
O. S. Wenger

Flipper changes in the donor and acceptor [OC-124]

Nerea Gonzalez-Sanchis, University of Geneva
N. Sakai, S. Matile

Three- and One-Dimensional Assembly of π -Aromatics for Photo- and Redox-Active Organic Materials [OC-125]

Philip Hope, University of Zurich
S. McGonigal, M. Rickhaus, A. Avestro

Self-sorting collagen heterotrimers [OC-126]

Valdrin Islami, ETH Zurich
P. Bittner, N. B. Hentzen, R. Zenobi, H. Wennemers

pH-Dependent Stoppering of Rotaxanes via Electrostatic Attraction [OC-127]

Laurent Jucker, University of Basel
Y. Aeschi, M. Mayor

Cyclic Thiosulfonates for Thiol-Mediated Uptake: Cascade Exchangers, Transporters, Inhibitors. [OC-128]

Takehiro Kato, University of Geneva
B. Lim, Y. Cheng, A. Pham, J. Maynard, D. Moreau, A. I. Poblador-Bahamonde, N. Sakai, S. Matile

1,3,2-Diazaphospholene-Catalyzed Reductive Cyclizations of Organohalides [OC-129]

Johannes Klett, EPFL Lausanne
L. Woźniak, N. Cramer

Cycloparaphenylene double hoops as circularly polarized light emitters [OC-130]

Kovida Kovida, University of Bern
T. Šolomek

Stimuli-responsive molecular nanocarbons [OC-131]

Remigiusz Krecijasz, University of Bern
T. Šolomek

Enantiospecific Complexation of Planar Chiral Iridium and Rhodium Cyclopentadienyl Complexes and their Application in Catalysis [OC-132]

Aragorn Laverny, EPFL Lausanne
N. Cramer

Understanding aggregation formation during peptide synthesis using in-line UV analysis [OC-134]

Robin Lescure, University of Zurich
H. Bürgisser, B. Tamás, N. Hartrampf

Access to α -Chiral Olefin via Nickel-Catalyzed Enantio-convergent Cross-Coupling between β -Bromostyrenes and Secondary Grignard Reagents [OC-135]

Kaidi Li, University of Geneva
C. Mazet

Protecting-Group-Free Synthesis of 1,2-cis Glycosides using a Double Inversion Strategy [OC-136]

David Lim, University of Bern
F. Paradisi

Chiral Cyclic Alkyl Amino Carbene (CAAC) Transition-Metal Complexes: Synthesis, Structural Analysis and Evaluation in Asymmetric Catalysis [OC-138]

Adrien Madron du Vigné, EPFL Lausanne
N. Cramer

Unprotected 2-azidoamines from alkenes – Facile access to masked diamines by using stable N–O reagents [OC-139]

Szabolcs Makai, ETH Zurich
E. Falk, B. Morandi

Emissive Properties of Helicene Carbon Nanohoops [OC-140]

Juraj Malinčík, University of Basel
S. Gaikwad, J. P. Mora-Fuentes, M. Boillat, A. Prescimone, D. Häussinger, A. G. Campaña, T. Šolomek

Unlocking Aluminum Reagents Towards Deprotonative Metalation Reactions [OC-141]

Xenia Meissner, University of Bern
E. Hevia

Synthesis of Tetrahydrooxepines via Ring Expansion of Medium-Sized Oxacycles [OC-142]

Claire Montagnon, University of Geneva
R. Pertschi, J. Lacour

N-Nitrosaccharin: Powerful Organic Reagent for Electrophilic Ipso-Nitration of Silanes [OC-143]

Ivan Mosiagin, University of Fribourg
D. Katayev

Direct Light Activation of Hypervalent Iodine Reagents: Substrate-Controlled C-C or C-H Alkynylation of Cyclopropanes. [OC-144]

Tin Nguyen, EPFL Lausanne
M. Wodrich, J. Waser

Aromatic C-H Insertions of Malonate Metal Carbenes for Late-Stage Functionalization of Diaza^[4] Helicenes [OC-145]

Yana Nikolova, University of Geneva
B. Fabri, P. Moneva Lorente, A. Guarnieri-Ibáñez, A. de Aguirre, F. Zinna, L. di Bari, A. Poblador-Bahamonde, J. Lacour

Functionalization of C²-C² bonds through earth abundant metal-catalysis [OC-146]

Pierre Palamini, EPFL Lausanne
E. M. D. Allouche, J. Waser

Electrocatalytic Activation of Ferric Nitrate [OC-147]

Subrata Patra, University of Fribourg
D. Katayev

A Concise Total Synthesis of the ABO Blood Antigens [OC-148]

Keir Penston, University of Bern
D. Lim, F. Paradisi

Nickel-Catalyzed Kumada Vinylation of Enol Phosphates: A Comparative Mechanistic Study [OC-149]

Philippe-Alexandre Poisson, University of Geneva
G. Tran, C. Besnard, C. Mazet

Radical Iodo- and Hydroalkylation Modification of Forskolin [OC-150]

Elena Pruteanu, University of Bern
N. D. Tappin, V. Gîrbu, O. Morarescu, F. Dénès, V. Kulcički, P. Renaud

Stereoselective Peptide Catalysis in Complex Environments – From River Water to Cell Lysates^[1] [OC-151]

Jonas Rackl, ETH Zurich
T. Schnitzer, H. Wennemers

Insights into the Molecular Mechanism of Cobalt(II) Catalyzed C-O cross-Coupling Reaction: A DFT study [OC-152]

Chandralekha Rajalakshmi, CMS College Kottayam

Enantioselective 3-Component Reaction between Hypervalent Iodine Reagents, Fluorinated Diazo Compounds and Nucleophiles [OC-153]

Nieves Ramirez, EPFL Lausanne
J. Waser

Activation of amino monoester strained rings with silylium catalysis [OC-154]

Emma Robert, EPFL Lausanne
V. Pirenne, J. Waser

Pd(II)-Catalyzed Aminoacetoxylation of Alkenes via Tether Formation [OC-155]

Thomas Rossolini, EPFL Lausanne
A. Das, S. Nicolai, J. Waser

Overcoming Catalyst Deactivation: Access to Fluorinated γ -Nitroaldehydes by Peptide Catalysis [OC-156]

Martin Schnurr, ETH Zurich
H. Wennemers

Digitalization and optimization of enantioselective multicomponent reactions [OC-157]

Alexandre Schöpfer, EPFL Lausanne
N. P. Ramirez, R. Laplaza, P. van Gerwen, J. Waser, C. Corminboeuf

Radical Mediated Hydroperfluoroalkylation of Unactivated Alkenes [OC-158]

Gulsana Sissengaliyeva, University of Bern
E. Pruteanu, F. Dénès, P. Renaud

Synthesis and applications of novel chiral monophosphine ligands [OC-159]

Vitalii Smal, EPFL Lausanne
A. Vorobei, D. Maye, N. Cramer

Radical azidation of cyclopropenes towards synthesis of quinolines [OC-160]

Vladyslav Smyrnov, EPFL Lausanne
B. Muriel, J. Waser

Defined “patches“ of interwoven materials [OC-161]

Luise Sokoliuk, University of Basel

Anion- π Catalyzed Ether Cascade Cyclization in Vesicles [OC-162]

Meiling Tan, University of Geneva
H. Chen, M. Gutiérrez López, N. Sakai, S. Matile

Tailoring Sodium Organometallic Reagents for Arene Functionalization [OC-163]

Andreu Tortajada, University of Bern
E. Hevia

Carpyridine sheets: shape (and size) matters! [OC-164]

Joseph Woods, University of Zurich
L. Gallego, P. Pfister, M. Maaloum, A. Vargas Jentzsch, M. Rickhaus

At the Core of Dynamic Polymers: The Self-Assembly of Twisted Aryl Amines [OC-165]

Kai Zhang, University of Zurich
M. Nehme, M. Rickhaus

Physical Chemistry [PC]**Poster Session****Synthesis and structural determination by X-ray crystallography of metal nanoclusters [PC-101]**

Khadijetou Ahmed Ethmane, University of Geneva
A. Rosspeintner, E. Bordignon, T. Bürgi, C. Besnard

Unravelling the Mass Transport of Water at Organic Aerosol Interfaces [PC-102]

Mercede Azizbaig Mohajer, ETH Zurich
M. J. Gleichweit, F. Graber, R. Signorell

Cold ion-molecule reactions between He⁺ and small molecules with a quadrupole moment [PC-103]

Fernanda B V Martins, ETH Zurich
F. van Swaaij, V. Zhelyazkova, F. Merkt

Nanoscale Analysis of On-Surface Coordination Systems Using Tip-Enhanced Raman Spectroscopy [PC-105]

Zhen-Feng Cai, ETH Zurich
Z. Cai, L. Zheng, Y. Zhang, R. Zenobi

High-resolution spectroscopy of metastable helium atoms using beam-manipulation methods [PC-106]

Gloria Clausen, ETH Zurich
L. Gabriel, J. A. Agner, H. Schmutz, F. Merkt

Enhanced stability and solubility of photoacids in binary solvent mixtures [PC-107]

Anna de Vries, ETH Zurich
M. Reiter, K. Goloviznina, M. Salanne, M. R. Lukatskaya

Zero-quantum-defect method using the Stark effect in Rydberg states of para-H₂ [PC-108]

Ioana Doran, ETH Zurich
N. Hölsch, F. Merkt

Probing Photocatalytic Reactions at the Single-particle and Single-photon Level [PC-109]

Leon Feld, ETH Zurich
G. Rainò, Y. Sahin, D. Dirin, M. V. Kovalenko

Polaritonic chemistry with instanton theory [PC-110]

Marit Fiechter, ETH Zurich
J. O. Richardson

Phosphate ion triggered modifications of oil/water interfaces [PC-111]

Matteo Frigerio, University of Fribourg
S. Salentinig

Femtosecond broadband spectroscopic study of planarization dynamics of 9,10 -bis(phenylethynyl)anthracene [PC-112]

Ina Fureraaj, University of Geneva
D. S. Budkina, E. Vauthey

Fabrication of nano-masked test samples for chemical etching relevant to microchip fabrication: An electron beam lithography approach [PC-113]

Liliana Galvez-Vazquez, University of Bern
P. Moreno Garcia, M. Galvez Vazquez, P. Broekmann

Electrolyte engineering for Zn-ion batteries: Concentration-dependent Zn₂⁺ coordination structure and its implication on Zn metal anode reversibility [PC-114]

Dario Gomez Vazquez, ETH Zurich
J. Yoo, O. Borodin, T. P. Pollard, J. Mars, H. Steinrück, S. E. Bone, M. Lukatskaya

Quantifying London Dispersion Interactions in Onium Ions [PC-115]

Vladimir Gorbachev, ETH Zurich
A. Savoy, L. Fritsche, P. Chen

Energy-dependence of reactions of D₂⁺ + NH₃ and D₂⁺ + CH₃F [PC-116]

Raphaël Hahn, ETH Zurich
J. Agner, H. Schmutz, F. Merkt

Methodological and Instrumental Developments in Improving the Resolution Limit of PFI-ZEKE Photoelectron Spectroscopy [PC-117]

Holger Herburger, ETH Zurich
V. Wirth, U. Hollenstein, F. Merkt

Polymer GUVs for High-Throughput Screening [PC-118]

Lukas Heuberger, University of Basel
C. G. Palivan

IDTBT polymers studied with in-situ time-resolved spectro-electrochemistry [PC-119]

Isabelle Holzer, University of Bern
P. Cavassin, N. Banerji

DNP-enhanced NMR of Passivating Agents on Hybrid Perovskite Thin Films [PC-120]

Michael Hope, EPFL Lausanne
A. Mishra, L. Emsley

Laser Cooling of Ions in Strongly Inhomogeneous Magnetic Fields [PC-121]

Richard Karl, University of Basel
Y. Yin, S. Willitsch

QCL Dual-Comb Spectrometer Measurements of cold CHCl₃F and CF₄ [PC-122]

Karen Keppler, ETH Zurich
J. A. Agner, S. Albert, P. Allmendinger, U. Hollenstein, A. Hugi, P. Jouy, M. Mangold, F. Merkt, M. Quack

Inverting glucuronidation of hymecromone in situ by catalytic nanocompartments [PC-123]

Maria Korpidou, University of Basel
V. Maffei, I. Dinu, C. Schoenenberger, W. P. Meier, C. G. Palivan

High-resolution spectroscopy of the ground state of MgK⁺ and its low-lying electronically excited states [PC-124]

Carla Kreis, ETH Zurich
M. Holdener, M. Génévriez, F. Merkt

Combined electrochemical and thermochemical approach to determine the fundamental reaction processes of the CO₂ reduction reaction [PC-125]

Paul Leidinger, Paul Scherrer Institut, Villigen
T. J. Schmidt, J. A. van Bokhoven, J. A. van Bokhoven, J. Herranz, L. Artiglia

Investigations on the chemical behavior of cesium and iodine in lead-bismuth liquid metal solution [PC-126]

Lu Liu, Paul Scherrer Institut, Villigen
Zivanovic, E. Karlsson, D. Herrmann, A. Vögele, J. Neuhausena

Super-Resolution Microscopy with Mechanosensitive Membrane Tension Probes [PC-127]

Jimmy Maillard, University of Geneva
E. Drab, J. Garcia-Calvo, N. Sakai, S. Matile, A. Fürstenberg

Cation Dynamics in Hybrid Perovskites from Solid-state NMR Spectroscopy [PC-128]

Aditya Mishra, EPFL Lausanne
M. A. Hope, M. Cordova, L. Emsley

Studying rotational-state and conformational effects in chemi-ionisation reactions [PC-129]

Amit Mishra, University of Basel
L. Ploenes, P. Straňák, S. K. Kim, S. Willitsch

Leaded bronze foams: a novel high surface area electrocatalyst material for cathodic electrosynthesis [PC-130]

Pavel Moreno-García, University of Bern
T. Prenzel, M. Gálvez-Vázquez, L. Gálvez-Vázquez, S. R. Waldvogel, P. Broekmann

The Structure of Water in No Man's Land [PC-131]

Nathan Mowry, EPFL Lausanne
C. Krüger, M. Drabbels, U. J. Lorenz

Vibrational Spectroscopy of New Molecular Probes for Interfacial Sensing [PC-132]

Mariano Parra, University of Zurich
B. Dereka

Prediction of mycotoxin response of DNA-wrapped nanotube sensor with machine learning [PC-133]

Yahya Rabbani, EPFL Lausanne
S. Behjati, B. Lambert, S. Sajjadi, M. Shariaty-Niassar, A. A. Boghossian, A. A. Boghossian

Precision spectroscopy and coherent manipulation of single trapped molecular N_2^+ ions [PC-134]

Mikołaj Roguski, University of Basel
A. Shlykov, M. Sinhal, R. Karl, P. Paliwal, S. Willitsch

2DRaman-THz spectroscopy with single-shot THz detection [PC-135]

Saurabh Shukla, University of Zurich
M. Duchi, A. Shalit, P. Hamm

Photoinduced Electron Transfer in a Porphyrin-Fullerene Dyad at a Liquid Interface [PC-136]

Jihad Sissaoui, University of Geneva
A. Efimov, T. Kumpulainen, E. Vauthey

A cryogenic hybrid trap for cold ion-molecule reactions [PC-137]

Pietro Vahramian, University of Basel
C. Von Planta, D. Haas, C. Mangeng, R. Karl, D. Zhang, T. Kierspel, Y. Ying, S. Willitsch

Bimolecular Photoinduced Electron Transfer in Non-Polar solvents [PC-138]

Pragya Verma, University of Geneva
E. Vauthey

Femtosecond laser-induced fragmentation mechanism of gold nanoparticles in water [PC-139]

Chengcheng Yan, EPFL Lausanne
G. Bongiovanni, P. K. Olshin, J. M. Voss, M. Drabbels, U. J. Lorenz

A generalised-dividing-surface diabatic instanton rate theory [PC-140]

Rhiannon Zarotiadis, ETH Zurich
J. O. Richardson

Ion-molecule reactions near 0K: the effect of the unpaired electron in NO on the He^+ + NO reaction rate coefficients [PC-141]

Valentina Zhelyazkova, ETH Zurich
F. B. Martins, S. Schilling, F. Merkt

Performance of chemoresistive nanosensors in the detection of gas-phase impurities after irradiation with gamma-rays and alpha particles. [PC-142]

Giulia Zonta, University of Ferrara
M. Astolfi, S. Gherardi, C. Malagù, M. Kasprzak, P. Steinegger, N. M. Chiera

Single molecular insights into receptor binding energetics of SARS-CoV2-variants [PC-143]

Ankita Ray, Université catholique de Louvain
M. Koehler, R. Moreira, B. Juniku, A. Poma, D. Alsteens

**Polymers, Colloids & Interfaces [PI]
Poster Session****Photo-crosslink bottlebrush polymers for voltage-driven artificial muscles [PI-101]**

Yeerlan Adeli, EPFL Lausanne/Empa
F. Owusu, F. A. Nüesch, D. M. Opris

Selective Removal of Toxic Organic Dyes using Troeger Base Containing Sulfone Copolymers made from a Meta-Free Thiol yne Click Reaction Followed by [PI-102]

Bassam Alameddine, Gulf University for Science and Technology
N. Baig, S. Shetty

Stimuli-responsive, functional, porous membranes for ultrafast and switchable gas separation applications [PI-103]

Timur Ashirov, University of Fribourg

Lipidic mesophases for local delivery of rapamycin to treat inflammation [PI-104]

Gregor Bordon, University of Bern
S. Aleandri, M. Carone, P. Luciani

An Approach to Photoredox Catalysis Using Light-Harvesting Supramolecular Polymers [PI-105]

Romain Brisse, University of Bern
S. Langenegger, S. X. Liu, R. Häner

Hydrogel-liposome composite for local treatment of fibrosis [PI-106]

Marianna Carone, University of Bern
S. Teworte, S. Aleandri, G. Bordon, P. Luciani

Characterization of a hydrophobic PEDOT derivative using eQCM [PI-107]

Polyxeni Damala, University of Geneva
E. Bakker

All solvent-free synthesis of dielectric elastomer transducers [PI-108]

Patrick Danner, Empa
D. M. Opris

Thermo-responsive smart gating wood membranes [PI-109]

Yong Ding, ETH Zurich
G. Panzarasa, S. Stucki, T. Keplinger, I. Burgert

Assembly of functionalized supramolecular polymers [PI-110]

Edouard Ehret, University of Bern
S. M. Langenegger, R. Häner

Characterisation of New Self-Plasticised Redox Polymer based on 3,4-Ethylenedioxythiophene [PI-111]

Tara Forrest, University of Geneva
E. Bakker

Development and characterization of a pH-responsive lipid-based nutrient delivery vehicle [PI-112]

Parth Kadakia, University of Fribourg
S. Salentinig

Towards Self-Regulation in Polymeric Microactuators [PI-113]

Michael Lerch, University of Groningen
S. Li, B. Deng, J. T. Waters, A. C. Balazs, J. Aizenberg

A modular silica core-shell synthesis particle platform: rough, sticky and yet reversible colloidal gels. [PI-114]

Florence Müller, ETH Zurich
L. Isa, J. Vermant

Union Carbide Polymerization Catalysts: from Uncovering Active Site Structures to Designing Molecularly-Defined Analogs [PI-115]

Anna Nobile, ETH Zurich
D. Trummer, P. Payard, A. Ashuiev, Y. Kakiuchi, D. Klose, G. Jeschke, C. Copéret

Interpenetrated Elastomeric Networks containing Supramolecular Motifs [PI-116]

Ilaria Onori, University of Fribourg
J. A. Berrocal, C. Weder, J. A. Berrocal

Insights into Engineered Protein Condensates and their Applications [PI-117]

Florence Stoffel, ETH Zurich
A. Küffner, U. Capasso Palmiero, L. Faltova, P. Arosio

Supramolecular Self-Assembly of Pyrene-DNA Conjugates into Vesicles [PI-118]

Jan Thiede, University of Bern
S. M. Langenegger, R. Häner

Reversing RAFT Polymerization: Near-Quantitative Depolymerization into Monomer via a Catalyst-Free Approach [PI-119]

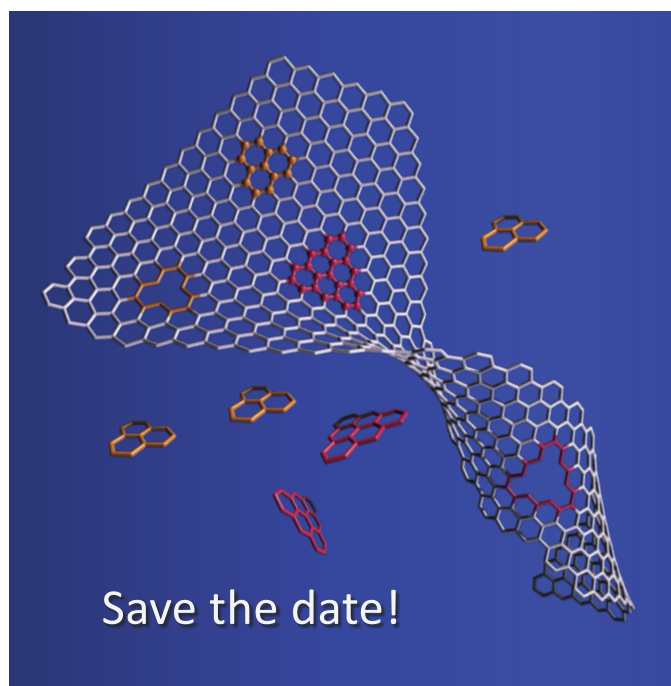
Hyun Suk Wang, ETH Zurich
N. P. Truong, Z. Pei, M. L. Coote, A. Anastasaki

In situ Characterization of Viruses Colloidal Systems for Design of Antiviral Solutions [PI-120]

Samuel Watts, University of Fribourg
S. Salentinig

Novel Polyphosphazenes for Dielectric Elastomer Applications [PI-121]

Cansu Zeytun Karaman, EPFL Lausanne
F. Nüesch, D. M. Opris

**SCS Fall Meeting 2023**

University of Bern, VonRoll Campus

Monday, August 24, 2023, 13.00-21.00h

- Helvetica Session
 - 2 Invited lectures
- «Young Leaders on Stage»
 - 3 Parallel sessions for Postdocs and PIs
- Excellence in Swiss R&D
 - 3 Invited lectures
- ChemEdu 2023
 - Symposium Future of Chemical Education
- Beer & Brezel Party and poster session A

Tuesday, August 25, 2023, 08.30-19.30h

- 2 Plenary sessions with lectures of the SCS award winners 2023
- 2x 9 Parallel sessions with invited lectures and PhD short talks
- Poster session B and commercial exhibition
- Award ceremonies

Call for contributions open from January 15 to May 15, 2023, on fm23.scg.ch

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Artwork by
Dr Lenka Štacková,
University of Zurich

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