



SCS
Swiss Chemical
Society

Online Conference

Friday, 10. September 2021, 09:15-18.30

SCS Fall Meeting 2021

- SCS award lectures in two plenary sessions
- Lectures by invited speakers
- PhD short presentations in 9 parallel sessions
- Whole week virtual poster sessions
- Best presentation awards (Metrohm/DSM prizes)

Registration is free for SCS Members

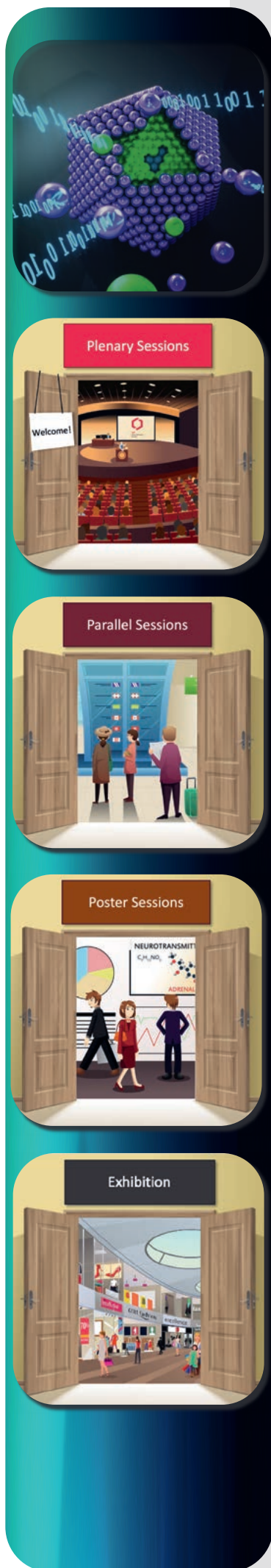
Non-members can register online until the start of the conference. As of August 16, we will only accept payment by credit card.

fm21.scg.ch

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**UNIVERSITÄT
BERN**

Fall Meeting main graphic (picture on the top):
Raffaella Buonsanti, Laboratory of Nanochemistry for Energy,
EPFL Valais Wallis, Sion



WELCOME TO THE 2021 FALL MEETING OF THE SWISS CHEMICAL SOCIETY (SCS)



Prof. Eva Hevia

On behalf of the Organizing Committee and the board members of all involved SCS Networks, we welcome you to the 2021 Fall Meeting, again held as a virtual meeting & virtual exhibition.

To be honest, we all are eagerly awaiting the moment on-site meetings will be possible again. This fall, after a long break due to the pandemic, the SCS is again holding smaller events as on-site events, but for large events, the risk and planning uncertainty are still too high. EPFL, the designated host of the Fall Meeting 2021, signaled already at the beginning of the year that no large events would be possible at the campus in Lausanne. Given the positive experience from the 2020 event,^[1] we decided to hold the Fall Meeting again as a virtual conference. Again, as in the previous year, we could count on the support of the Department of Chemistry, Biochemistry and Pharmaceutical Sciences of the University of Bern for running the 'operation center'.



Dr. Hans Peter Lüthi

Even though they are not a full replacement for on-site conferences, online events also offer certain advantages. For example, virtual posters in the form of short videos, as introduced at the 2020 Fall Meeting, are now well established. Being on display for a longer period makes it possible to study contributions even before and after the conference. Zoom as platform for lectures and presentations is also fully accepted, but the lack of virtual 1:1 interaction was considered the feature missed most. To fill this gap, the Fall Meeting 2021 goes new ways and organizes the lunch break including the poster sessions using Gather.Town. This tool offers the opportunity to communicate directly with other participants *via* video chat. Even though we have already gained experience with the platform at a few smaller SCS symposia, we have never used it for such a large event. We are very much looking forward to it, however, to be honest we are also a bit nervous. But we accept the challenge!



David Spichiger

The fact that the Fall Meeting is also an important platform for the community in virtual form is demonstrated by the more than 450 abstracts submitted. 112 oral contributions and almost 350 posters await the participants.

Our Fall Meeting online conference platform offers four virtual rooms:

- In the 'Plenary Session Room', you can follow the Award Lectures (Werner and Sandmeyer Prizes and the Industrial Science Awards).
- The 'Parallel Sessions Room' offers the platforms for the nine thematic sessions, most with two Invited Lectures and ten Short Talks presented by students.
- The 'Virtual Posters' room is accessible during the entire week. On September 10, during lunch time, you can interact with the presenters on a 1:1 basis *via* Gather.Town.
- In the 'Exhibition Room' you can visit the booths of our exhibitors. All exhibitors are also part of the Gather.Town virtual space.

The meeting ends with the announcement of the winners of the 'SCS Helvetica Prize' and the award ceremony, honoring the Best Oral and Best Poster Presenters. This award program is one of the best endowed worldwide, and the ceremony is always one of the highlights of the event.

We gratefully acknowledge the generous support of our sponsors, some of whom have been with us for many years. We thank all the members of the Organizing Committee for setting up attractive session programs. We invite you to browse through the program and look forward to meeting you in the virtual rooms and online platforms of the 2021 Fall Meeting.

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

Prof. Eva Hevia
Chair of the
Organizing Committee

David Spichiger
SCS Executive Director

[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, FRIDAY, 10TH SEPTEMBER 2021

Interactive program incl. abstracts of all lectures, talks and virtual posters on <https://fm21.scg.ch>

Time	Program Item
08.30	Open virtual conference room
09.15	Welcome and conference opening <i>Prof. Eva Hevia</i> , University of Bern and <i>Dr. Hans Peter Lüthi</i> , SCS Foundation Co-Chairs of the SCS Fall Meeting 2021
Morning Plenary Session (Award Lectures) – Chair Alain De Mesmaeker	
09.30	Sandmeyer Award Lecture 2021 <i>Dr. Pierdomenico Biasi</i> , Casale SA and <i>Dr. René Eckert</i> , Clariant Produkte (Deutschland) GmbH «AmoMax®-Casale: from the concept to the implementation in industrial reactors»
10.10	SCS Industrial Science Award Lecture 2021 <i>Dr. Cornelia Zumbunn</i> , Idorsia Pharmaceuticals Ltd, «A Battle for New Antibiotics»
10.50	Short Break
Morning Parallel Sessions	
11.00	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 and Polymers, Colloids & Interfaces
Lunch Break and Poster Session	
12.45	Virtual Poster Sessions Read abstracts, watch short videos and interact with the presenters <i>via</i> Gather.Town. The poster session is open from Mon, 06.09.2021 to Fri, 17.09.2021. Virtual Commercial Exhibition Visit the virtual booths and inform yourself about the latest developments of our partners Participate in the online quiz and get the chance to win 100 and 2x 50 CHF in cash.
13.45	General Assembly of the youngSCS 2021 Lead: Benjamin Ries, 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 and Polymers, Colloids & Interfaces
16.15	Short Break
Afternoon Plenary Session (Award Lectures) – Chair Alain De Mesmaeker	
16.30	Werner Prize Lecture 2021 <i>Prof. Raffaella Buonsanti</i> , EPFL Lausanne, «Mechanistic insights into the formation of Cu nanocrystals pave the way towards better catalysts to reduce CO ₂ »
17.10	SCS Senior Industrial Science Award Lecture 2021 <i>Dr. Andrew Edmunds</i> , Syngenta Crop Protection AG, «Some Highlights from an Agro Career»
SCS Announcements and Ceremony Session	
17.50	SCS Announcements Helvetica Prize of the Swiss Chemical Society 2021 (best published papers of PhD/Postdocs 2020/21)
18.00	Best Oral Presentation Awards (sponsored by Metrohm) Dipl. Ing. Markus Steinke, Executive Vice President Marketing at Metrohm Best Poster Presentation Awards (sponsored by DSM) Dr. Werner Bonrath, DSM Nutritional Products
18.30	End of the conference

GENERAL INFORMATION

Date: September 10, 2021, 09.15–18.30 h
 Location: Online Meeting
 Host: University of Bern, Department of Chemistry, Biochemistry and Pharmaceutical Sciences
 Website: <https://fm21.scg.ch/>

Conference Secretariat

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

Organizing Committee

Chairs

Prof. Eva Hevia
 Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern
eva.hevia@unibe.ch
 Dr. Hans Peter Lüthi
 ETH Zürich and SCS Foundation
luethi@scg.ch

Session Chairs

Analytical Sciences
 – Dr. Ksenia Groh, Eawag Dübendorf
 – Dr. Hanspeter Andres, Federal Institute of Metrology, METAS

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 Zürich
 – Prof. Jeremy Richardson, ETH Zürich

Inorganic & Coordination Chemistry

– Prof. Marinella Mazzanti, EPF Lausanne
 – Prof. Kay Severin, EPF Lausanne
 – Prof. Roger Alberto, University of Zürich

Organic Chemistry

– Prof. Pablo Rivera-Fuentes, EPF Lausanne
 – Prof. Jason Holland, University of Zürich
 – Prof. Michal Juriček, University of Zürich

Medicinal Chemistry & Chemical Biology

– Dr. Fides Benfatti, Syngenta Crop Protection AG
 – Prof. Jean-Louis Reymond, University of Bern

Physical Chemistry

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

Polymers, Colloids & Interfaces

– Prof. Esther Amstad, EPF Lausanne
 – Dr. Kuljeet Kaur, EPF Lausanne

Chemistry and the Environment

– Prof. Kathrin Fenner, Eawag Dübendorf and University of Zurich
 – Dr. Jutta Hellstern, Novartis
 – Dr. Stefan Höger, IES Ltd

Registration

Fees for presenters (poster or talk)

- SCS Members: free of charge (by convention the first name in the abstract author list)
- Non-members: CHF 250.00 (incl. VAT)

Fees for participants without a presentation

- SCS Members: free of charge. However, registration is mandatory.
- Non-members: CHF 100.00 (incl. VAT)
 Participants who register after August 16 will have to pay the fees by credit card during the registration process.
 Registration is mandatory (also for SCS members) to access the virtual conference. Please proceed accordingly on our website.

Access the Virtual Conference

Select the menu item ‘Online Conference’ on the conference website to open the entry point for the lecture sessions, the poster sessions and the exhibition.

While the exhibition is accessible without a login attending the scientific sessions needs a participant profile.

Platform for the Lectures

All lectures and information sessions will be provided *via* Zoom video platform. To profit from the full functionality of the tool we recommend downloading and installing the *Zoom Client* on your device. For more details please go the website:

zoom.us/download#client_4meeting

Virtual Poster Sessions / Short videos

Poster presenters introduce their research project in short videos of 3 minutes. With this approach it's easier for the audience to follow numerous presentations and to understand the key message of each project. Tools to interact with the presenter allow visitors to ask questions or to comment the presented content. We offer email, skype or social media channels to interact with each other. On September 10, during lunch time, the poster session will take place on Gather.Town, an interactive conference platform.

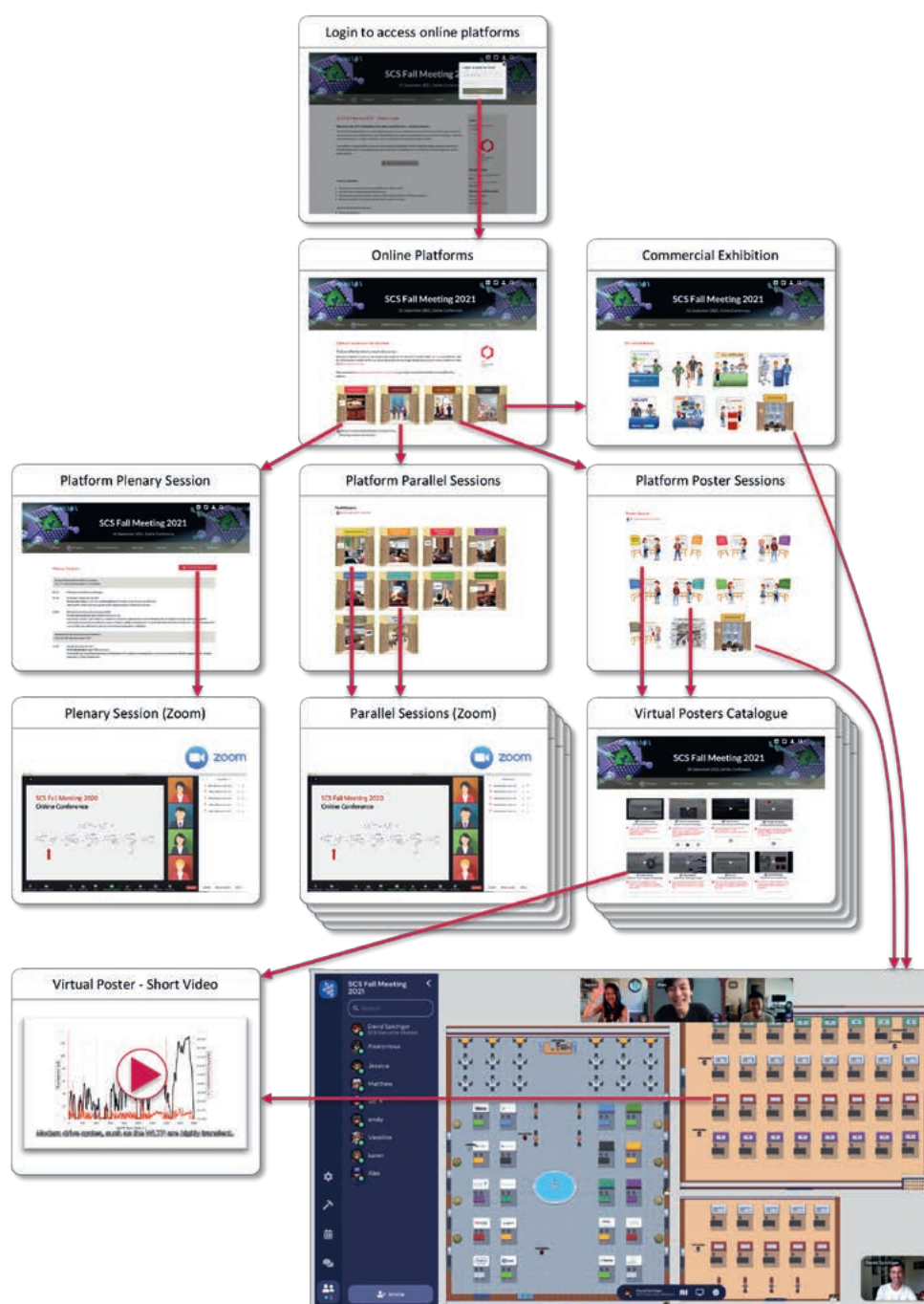
Program and Abstract Search

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

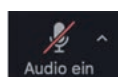
- Interactive program overview with abstract preview
- Quick abstracts display as html file
- pdf-file download of single abstracts
- Extensive search functionalities
- Interaction with the poster presenters *via* email or social media channels.

The screenshot displays the SCS Fall Meeting 2021 website interface. At the top, there is a navigation bar with options like Home, Program, Online Conference, Abstracts, Contacts, and Registration. Below this, a 'Schedule of SCS Fall Meeting 2021' table is visible, listing sessions by start time and topic. A specific session titled 'Methanol synthesis via hydrogenation of hybrid CO₂/CO feeds' is highlighted with a red box and a number '3'. To the right, a detailed abstract preview for this session is shown, including the title, authors, a brief description of the research, and a figure showing the reaction scheme and performance metrics. A number '4' is placed in a box next to the abstract preview. The interface also includes a search bar and a 'Filter' button for abstracts.

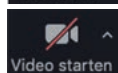
VIRTUAL CONFERENCE LOCATION



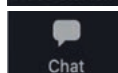
Rules for the online Lectures



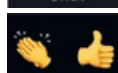
Audio on only for the speaker.
This function is managed by the operator



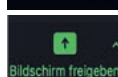
Deactivate the video function to reduce data transition.



Send your question *via* chat to the speaker or
send a note to the operator that you would like to ask a question in the Q&A session at the end of each presentation



Honor the speakers with your virtual applause at the end of each presentation



Sharing the screen is active for chairs and speakers only.
This function is managed by the operator.



Joining a session is allowed for registered participants only. Do not forward the meeting link and the password to third parties.

BEST PRESENTATION AWARDS

The organizers are proud of the very attractive presentation award program. Almost CHF 50'000 CHF in total are given to the winners in monetary form, travel grant or free publication opportunities in the Junior Laureates issue of CHIMIA 4/2022.

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 two best short presentations of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 18.00 h 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/short video of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 18.15 h in the plenary lecture room.

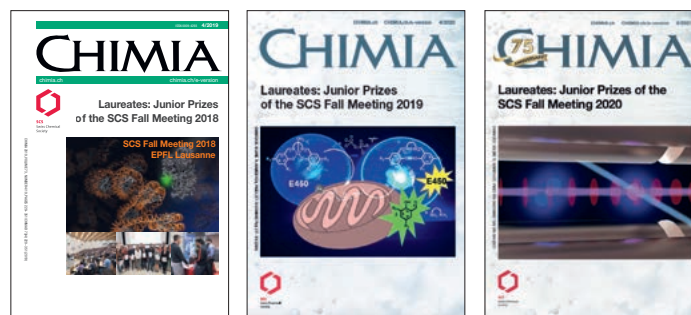
Prize for the winner of each of the nine poster session

- 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

- 2x cash contribution of CHF 200.

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 2019–2021 Junior Laureates Issues

Winners of the Best Presentation Awards 2020



HELVETICA PRIZE OF THE SWISS CHEMICAL SOCIETY 2021



Helvetica and the Swiss Chemical Society are proud to award the winners of the Helvetica Prize 2021 of the Swiss Chemical Society for the best published papers of PhD/Postdocs 2020/21 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 then present their papers in a 3min short presentation.

1st Prize: *Daniel Hernandez-Valdés*

(University of Zürich, Group of Prof. Roger Alberto)
«CO₂ to CO: Photo- and Electrocatalytic Conversion Based on Re(I) Bis-Arene Frameworks: Synergisms Between Catalytic Subunits»

DOI: <https://doi.org/10.1002/hlca.202000147>

2nd Prize: *Nadja E. Niggli*

(University of Basel, Group of Prof. Olivier Baudoin)
«Design of Chiral NHC-Carboxylates as Potential Ligands for Pd-Catalyzed Enantioselective C–H Activation»

DOI: <https://doi.org/10.1002/hlca.202100015>

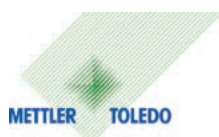
SPONSORS AND SUPPORTERS OF THE SCS FALL MEETING

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 Supporters



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



Physical Chemistry



Polymers, Colloids & Interfaces

COMMERCIAL EXHIBITORS



anton-paar.com/



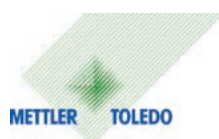
bachem.com



buchiglas.com



gmp.ch



ch.mt.com/



shimadzu.ch



mdpi.com



www.thieme.de



Visit our virtual exhibition and participate in the online quiz. Get the chance to win 1x CHF 100.00 or 2x CHF 50.00. All submitted online forms with at least 80% correct answers will participate in the draw on September 10, 18:00h.

The quiz is open from August 20, 2021, to September 10, 2021, 14.30h.

PLENARY SESSIONS

Award Lectures in the Plenary Sessions

Chairs: Dr. Alain De Mesmaeker, SCS President
Prof. Christian Bochet, University of Fribourg,
SCS Vice-President

Sandmeyer Award Lecture 2021

«AmoMax®-Casale: from the concept to the implementation in industrial reactors» [PS-001]

September 10, 2021, 09.30–10.10 h



Dr. Pierdomenico Biasi, Mr. John D'

Alessandri, Mr. Ermanno Fillippi Mr. Sergio Panza, Casale SA and

Dr. Rene Eckert, Dr. Marvin Estenfelder, Dr. Stephan Reitmeier, Dr. Andreas Reitzmann, Clariant AG

The team is awarded for the achievements obtained in the field of catalysis and reaction engineering, especially for the development and implementation of the AmoMax®-Casale, a new catalyst for a greener and less energy consuming process for industrial large scale ammonia synthesis.

SCS Industrial Science Award Lecture 2021

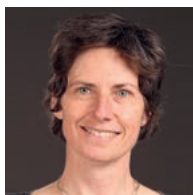
«A Battle for new Antibiotics» [PS-002]

September 10, 2021, 10.10–10.50 h

Dr. Cornelia Zumburrn

Idorsia Pharmaceuticals Ltd

The award is given to honor Cornelia's key contributions as a medicinal chemistry project leader in the challenging field of antibiotic drug discovery, including her contributions to several anti-bacterial research projects and the development of a significant number of chemical series into advanced compounds, some of which were ultimately selected as preclinical development candidates.



Werner Prize Lecture 2021

«Mechanistic insights into the formation of Cu nanocrystals pave the way towards better catalysts to reduce CO₂» [PS-003]

September 10, 2021, 16.30–17.10 h

Prof. Raffaella Buonsanti

EPFL Lausanne

Raffaella is honored for her original and significant contributions in the chemistry development of tailored nanomaterials and their applications in catalysis, especially CO₂ electroreduction.



SCS Senior Industrial Science Award Lecture 2021

«Some Highlights from an Agro Career» [PS-004]

September 10, 2021, 17.10-17.50h

Andrew Edmunds

Syngenta Crop Protection AG

Andrew receives this award in recognition of his impressive track record of achievements in the field of chemistry and crop protection reflected in 140 patents, 28 publications and more than 20 lectures at universities and international conferences.



Award Lectures as Contributed Lectures in the Parallel Sessions

METAS Award Lecture 2021

«Analysis of clumped isotopes in nitrous oxide by laser spectroscopy: method development and first applications» [AS-017]

September 10, 2021, 12.30–12.45h

Session Analytical Sciences

Dr. Kristýna Kantnerová

EMPA Dübendorf



Kristýna is honored for her excellent and timely work in the field of metrology of clumped isotopes of nitrous oxides.

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

PARALLEL SESSIONS

Analytical Sciences [AS] Session
Endowment: Mettler Toledo

Chairs: Dr. Kensia Groh, Eawag, Dübendorf
Dr. Hanspeter Andres, METAS

- 11:00 **From Smart Methods to Smartphones: The Dunning-Kruger Effect hits Analytical Science [AC-011]**
Davide Bleiner, Empa Dübendorf
- 11:30 **Studies on a downward inductively coupled plasma time-of-flight mass spectrometer to analyze droplets carrying particles or cells [AS-013]**
Thomas Vonderach, ETH Zurich
V. Wyss*
- 11:45 **Particle-size-resolved elemental analysis of road dust coupling SMPS to ICP-MS [AS-014]**
Kevin Kraft, University of Zurich/ Empa
Y. Zhao, A. Wichser, J. Wang, D. Bleiner*
- 12:00 **High-throughput ion spectroscopy using Hadamard transform multiplexing and high-resolution ion mobility separations [AS-015]**
Vasylyatsyna, EPFL Lausanne
A. H. Abikhodr, T. R. Rizzo*
- 12:15 **A new approach for identifying positional isomers of glycans cleaved from monoclonal antibodies [AS-016]**
Irina Dyukova, EPFL Lausanne
A. Ben Faleh, S. Warnke, N. Yalovenko, V. Yatsyna, P. Bansal, T. R. Rizzo*
- 12:30 **Analysis of clumped isotopes in nitrous oxide by laser spectroscopy: method development and first applications [AS-017]**
Kristýna Kantnerová, Empa
B. Tuzson, L. Emmenegger, S. M. Bernasconi, J. Mohn
-
- 14:30 **Managing Change in Change Resistant Laboratories [AS-021]**
Christoph Jansen, Mettler Toledo
- 15:00 **Analysis of Protein Modification caused by low-temperature plasma treatment [AS-023]**
Alina Begley, ETH Zurich
I. Oganessian, R. Zenobi*
- 15:15 **Capacitive Readout of Ion-Selective Electrode by Electronic Control for High Precision Measurement [AS-024]**
Pitchnaree Kraikaew, University of Geneva
S. Sailapu, E. Bakker*
- 15:30 **Distance-Based Heparin Sensing using Optodes embedded in Agarose Gel [AS-025]**
Robin Nussbaum, University of Geneva
K. J. Robinson, Y. Soda, E. Bakker*
- 15:45 **A mechanistic study of ozone-led gasification on graphite by scanning tunneling microscopy [AS-026]**
Shaoxian Li, EPFL Lausanne
S. Huang, K. Agrawal*
- 16:00 **ORIGIN: Towards *in situ* Laser Desorption Mass Spectrometry of Amino Acids, PAHs and Lipids on Ocean Worlds [AS-027]**
Nikita Boeren, University of Bern
L. Schwander, K. Kipfer, N. F. Ligterink, P. Keresztes Schmidt, V. Grimaudo, M. Tulej, R. Lindner, P. Ehrenfreund, P. Würz*, A. Riedo*

Catalysis Sciences & Engineering [CE]

Session Endowment: Casale



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

- 11:00 **Selectivity Control in CO₂ Electroreduction through Rational Catalyst and Electrolyte Design [CE-011]**
Beatriz Roldan Cuenya, Fritz-Haber-Institute of the Max Planck Society
- 11:30 **Enhancement of power-to-gas *via* multi-catalyst reactors tailoring reaction rate and heat exchange [CE-013]**
Emanuele Moiola, Paul Scherrer Institute, Villigen
- 11:45 **Methanol synthesis *via* hydrogenation of hybrid CO₂-CO feeds [CE-014]**
Thaylan Pinheiro Araújo, ETH Zurich
A. H. Hergesell, D. Faust Akl, S. Buchele, J. A. Stewart, D. Curulla-Ferré, C. Mondelli, J. Pérez-Ramírez*
- 12:00 **Following the structure of copper-zinc-alumina across the pressure gap in carbon dioxide hydrogenation [CE-015]**
Arik Beck, ETH Zurich
M. Zabitskiy, M. A. Newton, M. Mirzakhani, M. G. Willinger*, J. A. van Bokhoven*
- 12:15 **The Role of Alloying in Highly Selective and Stable Propane Dehydrogenation Catalysts based on Silica-Supported Pt-Mn Particles Prepared via SOMC [CE-016]**
Lukas Rochlitz, ETH Zurich
C. Copéret*
- 12:30 **Suppression of water inhibition and thermal deactivation on Pd/Al₂O₃ during lean methane oxidation using oxygen dithering [CE-017]**
Maneka Roger, EPFL Lausanne
T. Franken, D. Ferri, O. Kröcher, D. Ferri*
-
- 14:30 **tbd [CE-021]**
Speaker from Casale, Casale SA
- 15:00 **Titanium hydride surfaces for ammonia synthesis [CE-023]**
Emanuel Billeter, Empa
Z. Lodziana, A. Borgschulte
- 15:15 **Piano-stool N-heterocyclic carbene iron complexes and the impact of ligand variation on hydrosilylation activity [CE-024]**
Pamela Nylund, University of Bern
M. Albrecht*
- 15:30 **Single-Atom Substitution in Two-Dimensional Molybdenum Carbide: Implications for Electrocatalysis [CE-025]**
Denis Kuznetsov, ETH Zurich
Z. Chen, P. Kumar, P. Abdala, A. Fedorov*, C. Müller*
- 15:45 **Photo- and Electrocatalysis with a Polymerised Water Reduction Catalyst [CE-026]**
Franziska Rahn, University of Zurich
B. Probst, R. Alberto*
- 16:00 **Mn(II) Phosphine-Amino-Phosphinites: A Highly Modular Class of Pincer Complexes for Enantioselective Transfer Hydrogenation of ketones [CE-027]**
Harikrishnan Jayaprakash, ETH Zurich
H. Grützmacher*

Computational and Theoretical Chemistry [CC]

Session Endowment: Idorsia



Chairs: Prof. Jeremy Richardson, ETH Zurich

- 11:00 **tbd [CC-011]**
Speaker tbd
- 11:30 **Microcanonical and finite-temperature ab initio molecular dynamics simulations on quantum computers [CC-013]**
Igor Sokolov, IBM Research Europe
P. Barkoutsos, L. Moeller, P. Suchsland, G. Mazzola, I. Tavernelli*
- 11:45 **Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry [CC-014]**
Thomas Weymuth, ETH Zurich
M. Reiher*
- 12:00 **AI guided synthesis of the GDB Chemical Space [CC-015]**
Amol Thakkar, University of Bern
J. Reymond*
- 12:15 **Neural networks meet non-covalent interactions: Chalcogen bonding in a solution [CC-016]**
Veronika Jurásková, EPFL Lausanne
F. Célerse, R. Laplaza, C. Corminboeuf*
- 12:30 **Osmotic transport at the aqueous graphene and hBN interfaces: scaling laws from a unified, first principles description. [CC-017]**
Gabriele Tocci, University of Zurich
M. Iannuzzi, L. Joly, R. Meissner
-
- 14:30 **Unravelling the Impact of Halogen Bonds in Medicinal Chemistry with QM calculations [CC-021]**
Christoph Sager, Idorsia Pharmaceuticals Ltd.
- 15:00 **Pushing the limits of the Density Matrix Renormalization Group: from vibrational spectroscopy to quantum dynamics [CC-023]**
Alberto Baiardi, ETH Zurich
M. Reiher*
- 15:15 **How important are the residual nonadiabatic couplings for an accurate simulation of nonadiabatic quantum dynamics in a quasidiabatic representation? [CC-024]**
Seonghoon Choi, EPFL Lausanne
J. Vaníček*
- 15:30 **Unravelling heavy-atom quantum tunnelling in spin transitions [CC-025]**
Eric Heller, ETH Zürich
J. O. Richardson*
- 15:45 **Δ SCF for Efficient Nonadiabatic Molecular Dynamics in Condensed Phase Systems [CC-026]**
Momir Malis, University of Zurich
S. Lubner*
- 16:00 **The Challenge of Accurate Computation of Two-Photon Absorption Properties of Organic Chromophores in the Condensed Phase [CC-027]**
Mingxue Fu, University of Geneva
T. S. Wesolowski*

Chemistry and the Environment [EV]

Session Endowment: Givaudan

Chairs: Dr. Jutta Hellstern, Novartis
Dr. Stefan Höger, IES Ltd

- 11:00 **Environmental Photochemistry of Anilines [EV-011]**
Kristopher McNeill, ETH Zurich
- 11:30 **Mechanistic implications of oxygen uncoupling in two Rieske non-heme iron dioxxygenases [EV-013]**
Charlotte Bopp, Eawag, Dübendorf
T. Vonderach, H. E. Kohler, T. B. Hofstetter*
- 11:45 **Reactive Oxygen Species (ROS)-A promising metric linking aerosol toxicity and human health [EV-014]**
Z. Zhang, University of Basel
- 12:00 **NMVO, CH₄ and NH₃ emissions of different silage-based diets for dairy cows at herd level [EV-015]**
David Steger, Empa
S. Schrade, M. Zähler, M. Hill, K. Zeyer, S. Reimann, F. Dohme-Meier*, J. Mohn*
- 12:15 **Absolute validation of a balloon-borne spectrometer for water vapor measurements in the upper atmosphere [EV-016]**
Simone Brunamonti, Empa
M. Graf, T. Bühlmann, C. Pascale, H. Looser, L. Emmenegger, B. Tuzson
- 12:30 **Cadmium remobilization during sediment resuspension can lead dissolved concentration exceeding EU water framework maximum [EV-017]**
Nicolas Layglon, University of Geneva
V. Lenoble, L. Longo, S. D'Onofrio, S. Mounier, J. Mullot, D. Omanović, C. Garnier, B. Misson
-
- 14:30 **Replacing the need for *in vivo* animal testing - the use of alternative *in vitro* assays for PBT screening of fragrance chemicals [EV-021]**
Heike Laue, Givaudan Schweiz AG
G. Sanders, K. Jenner, G. Kreutzer, A. Natsch
- 15:00 **Metabolomic Profiling and Toxicokinetics Modeling to Assess the Effects of the Pharmaceutical Diclofenac in the Aquatic Invertebrate *Hyalella azteca* [EV-023]**
Qiuguo Fu, Eawag, Dübendorf
A. Scheidegger, E. Laczko, J. Hollender, Q. Fu*
- 15:15 **Assessing biodegradation of commercial plastic mulches in Swiss soils [EV-024]**
Mattia Cerri, ETH Zurich
S. Arn, A. Manfrin, T. Bucheli, F. Widmer, M. Sander*, K. McNeill*
- 15:30 **Antibiotics and hormone steroids in Norwegian biogas digestate [EV-025]**
Astrid Nesse, Norwegian University of Life Sciences
S. G. Aanrud, J. L. Lyche, T. A. Sogn, R. Kallenborn
- 15:45 **Development of transient lithium-ion battery with a high-performance Cellulosic Separator [EV-026]**
Neeru Mittal, ETH Zurich
A. Ojanguren, N. Cavašin, E. Lizundia, M. Niederberger*
- 16:00 **Diformylxylose as a New Polar Aprotic Solvent Produced from Renewable Biomass [EV-027]**
Anastasiia Komarova, EPFL Lausanne
J. S. Luterbacher*

Inorganic & Coordination Chemistry [IC]

Session Endowment:
Chemspeed Technologies

Chairs: Prof. Roger Alberto, University of Zurich
Prof. Kay Severin, EPFL Lausanne

- 11:00 **Using Coordination Complexes to Inhibit Mitochondrial Calcium Uptake [IC-011]**
Justin Wilson, Cornell University, New York
J. J. Woods, N. P. Bigham, Z. Huang
- 11:30 **Fe(TMP)₂ – Synthesis, characterisation and tuneable reactivity of a new Fe(II) bis(amide) complex [IC-013]**
Lewis Maddock, University of Bern
M. Mu, M. Peñas de Frutos, M. García-Melchor, E. Hevia*
- 11:45 **Iron and Cobalt Nitrilimide Complexes: Transformations to Nitride and Isocyanamide Complexes via a Fleeting Diazomethanediide Intermediate. [IC-014]**
Sadig Aghazada, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
D. Fehn, F. W. Heinemann, D. Munz, K. Meyer*
- 12:00 **Delivery of a masked uranium(II) by an oxide bridged diuranium(III) for multi-electron transfer reactions [IC-015]**
Dieuwertje Modder, EPFL Lausanne
C. T. Palumbo, I. Douair, L. Xu, R. Scopelliti, L. Maron, M. Mazzanti*
- 12:15 **ALISI – Automated Light induced Synthesis of ⁸⁹Zr-Radiolabeled Antibodies for ImmunoPET [IC-016]**
Simon Klingler, University of Zurich
J. P. Holland*
- 12:30 **A Biomimetic Superreduced Iron-Sulfur Cubane and its Oxidized Analogues [IC-017]**
Liam Grunwald, ETH Zurich
D. Klose, M. Clemancey, G. Blondin, G. Jeschke, M. Würle, V. Mougel*
-
- 14:30 **What is more important to enable efficient cyber-physical systems – Digital Twins or the degree of automation in RnD labs? [IC-021]**
Rolf Gueller, Chemspeed Technologies AG
- 15:00 **Fully Solvated, Monomeric ReII Complexes: Insights into the Chemistry of [Re(NCCH₃)₆]²⁺ [IC-023]**
Robin Bolliger, University of Zurich
G. Meola, H. Braband, O. Blacque, L. Siebenmann, Q. Nadeem, R. Alberto*
- 15:15 **Can early lanthanide sandwich complexes be efficient single-molecule magnets? [IC-024]**
Moritz Bernhardt, ETH Zurich
M. D. Korzynski, B. Le Guennic, O. Cador, C. Copéret*
- 15:30 **Chemical investigation with exotic radionuclides [IC-025]**
Nadine Chiera, Paul Scherrer Institute, Villigen
R. Dressler, D. Schumann, R. Eichler
- 15:45 **DNA-ferrocene as two-step-mechanophore [IC-026]**
Emilie Jean-Pierre, University of Fribourg
M. Taskova, E. Janett, K. M. Fromm*, C. G. Bochet*
- 16:00 **New oxide group-9 transition metal superconductors in the filled-Ti₂Ni type structure [IC-027]**
Keyuan Ma, University of Zurich
R. Lefèvre, K. Gornicka, P. Verma, X. Zhang, T. Klimczuk, F. O. von Rohr

Medicinal Chemistry & Chemical Biology [MC]

Session Endowment: Janssen/Cilag

Chairs: Dr. Fides Benfatti, Syngenta Crop Protection AG
Prof. Jean-Louis Reymond, University of Bern

- 11:00 **SCS Division of Medicinal Chemistry & Chemical Biology (DMCCB): Activities 2021/22 and General Assembly 2021 [MC-011]**
Jean-Louis Reymond, University of Bern
- 11:15 **A Covalent Strategy to Develop Highly Selective Chemical Probes Targeting PI3K α [MC-012]**
Chiara Borsari, University of Basel
E. Keles, J. McPhail, A. Schäfer, M. Gstaiger, J. Burke, J. Burke, M. Wymann*
- 11:30 **Design of an internal salt bridge in zwitterionic SUCNR1-antagonists for improved oral exposure [MC-013]**
Juraj Velcicky, Novartis Pharma AG
N. Gommermann, P. Janser, S. Costesta, R. Wilcken, T. Wagner, R. Stringer, A. Littlewood-Evans, M. Haffke
- 11:45 **Discovery of a selective antitubercular small-molecule inhibitor targeting CoaBC [MC-014]**
Jeannine Hess, University of Cambridge
J. C. Evans, C. Spry, V. Mendes, C. Marchetti, H. I. Boshoff, T. Blundell, V. Mizrahi, A. G. Coyne, C. Abell*
- 12:00 **Gamma-Secretase Modulators (GSM) for the potential treatment of Alzheimer's Disease (AD); Novel phenyl bioisosteres [MC-015]**
Hasane Ratni, F. Hoffmann-La Roche
- 12:15 **Machine Learning Guides the Design of Non-Hemolytic Antimicrobial Peptides [MC-016]**
Alice Capecci, University of Bern
X. Cai, H. Personne, T. Köhler, C. van Delden, J. L. Reymond*
- 12:30 **Discovery of an orally active and selective ALK2 kinase inhibitor for the treatment of a rare genetic bone disease [MC-017]**
Thomas Ullrich, Novartis Pharma AG
L. Arista, N. Stiefl, C. Dekker, V. Head, I. Kramer, S. Guth
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- 14:30 **Cyclic Tetrapeptides as Next-Generation Remedies of Lead Poisoning [MC-021]**
Tagwa Mohammed, University of Zurich
M. Shoshan*
- 14:45 **The Discovery of Isocycloseram: a Novel Isoxazoline Insecticide [MC-022]**
Myriem El Qacemi, Syngenta Crop Protection AG
- 15:00 **Disruption of mitochondrial redox homeostasis by enzymatic activation of a trialkylphosphine probe [MC-023]**
Jade Nguyen, EPFL Lausanne
A. Tirla, P. Rivera-Fuentes*
- 15:15 **The Screening Compound Collection: A Key Asset for Drug Discovery [MC-024]**
Julien Hazemann, Idorsia Pharmaceuticals Ltd.
- 15:30 **Exploring the function of microtubule post-translational modifications by semi-synthetic tubulin [MC-025]**
Eduard Ebberink, EPFL Lausanne
S. Fernandes, G. Hatzopoulos, M. Velluz, N. Agashe, P. Gönczy, C. Aumeier*, B. Fierz*
- 15:45 **Acceleration of New Medicines with "Discovery Process Research" at Janssen [MC-026]**
Daniel Pippel, Janssen R&D
- 16:00 **HaloTag9: an engineered protein tag for fluorescence lifetime multiplexing [MC-027]**
Michelle Frei, Max Planck Institute for Medical Research
M. Tarnawski, J. Roberti, B. Koch, J. Hiblot, K. Johnsson*

Organic Chemistry [OC]

Session Endowment:
Syngenta Crop Protection



Chairs: Prof. Pablo Rivera-Fuentes, EPFL Lausanne
Prof. Jason Holland, University of Zurich

- 11:00 **Reagent, Ligand and Catalyst Design: A Three-fold Approach to Organic Synthesis [OC-011]**
Josep Cornella, Max-Planck-Institut für Kohlenforschung
- 11:30 **Asymmetric, visible light-mediated radical sulfinyl-Smiles rearrangement to access all-carbon quaternary stereocentres [OC-013]**
Cedric Hervieu, Universität Zürich
M. Kirillova, T. Suarez, M. Müller, E. Merino*, C. Nevado*
- 11:45 **Towards Sustainable Catalysis: Development of Chiral α -Diimine Iron Complexes for Asymmetric Cycloadditions of 1,3-Dienes [OC-014]**
Elena Braconi, EPFL Lausanne
N. Cramer*
- 12:00 **Möbius Carbon Nano hoops [OC-015]**
Juraj Malinčík, University of Basel
S. Gaikwad, M. Boillat, D. Häussinger, T. Šolomek*
- 12:15 **Tailoring a Sodium Amide (NaTMP) for Transition-Metal Free C-H Borylation of Arenes [OC-016]**
Leonie Bole, University of Bern
E. Hevia*
- 12:30 **TiCl₃-Mediated Synthesis of 2,3,3-Trisubstituted Indolenines: Total Synthesis of (+)-1,2-Dehydroaspidospermidine, (+)-Condyfoline, and (-)-Tubifoline [OC-017]**
Bastien Delayre, EPFL Lausanne
C. Piemontesi, Q. Wang, J. Zhu*
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- 14:30 **Homogeneous catalysis using stable cyclometalated complexes [OC-021]**
Tomas Smejkal, Syngenta Crop Protection AG
- 15:00 **Beyond transfer hydrogenation: Transfer hydroarylation by catalytic activation of strong C–C bonds [OC-023]**
Marius Lutz, ETH Zurich
V. C. Gasser, B. Morandi*
- 15:15 **Ethynylbenziodoxolones: Photocatalysis and Direct Excitation for Difunctionalisation and Deoxyalkynylation [OC-024]**
Stephanie Amos, EPFL Lausanne
D. Cavalli, F. Le Vaillant, S. Nicolai, J. Waser*
- 15:30 **Functionalization of zigzag graphene fragments: Tales of the unexpected [OC-025]**
Leoš Valenta, University of Zurich
P. Ribar, T. Rosa de Araujo, O. Blacque, T. Šolomek, M. Juriček*
- 15:45 **Catalyst Repurposing Sequential Catalysis [OC-026]**
Frederic Bourgeois, University of Basel
J. A. Medlock, W. Bonrath, C. Sparr*
- 16:00 **Palladium Catalysed Mild C–H Arylation of Arenes [OC-027]**
Jyoti Dhankhar, University of Zurich
E. G. Fernández, C. Dong, T. K. Mukhopadhyay, A. Linden, I. Čoric*

Physical Chemistry [PC] Session

Endowment: PMI Science



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

- 11:00 **How to Assess Reduced-Risk Products Faster Using a Chemical Reactivity-Directed Non-Targeted Screening Approach [PC-011]**
Helena Andrade, Philip Morris Products S.A.
A. Knorr, J. Sabaratnam, S. Sendyk, C. Goujon Ginglinger
- 11:30 **Red-emitting fluorophores as nanoscopic water sensors [PC-013]**
Jimmy Maillard, University of Geneva
A. Fürstenberg*
- 11:45 **Ion-dipole and ion-quadrupole interaction effects in ion-molecule reactions at collisional energies E_{coll} between 0 and 40k_B K [PC-014]**
Valentina Zhelyazkova, ETH Zurich
F. B. V. Martins, J. A. Agner, H. Schmutz, F. Merkt*
- 12:00 **Time dependent dynamics of nuclear spin symmetry and parity violation in dichlorodisulfane (ClSSCl) during and after coherent radiative excitation [PC-015]**
Gunther Wichmann, ETH Zurich
G. Seyfang, M. Quack*
- 12:15 **Understanding water dissociation on O-Cu(111) [PC-016]**
Harmina Vejjayan, EPFL Lausanne
R. D. Beck*
- 12:30 **Observation of optical confinement effects on the reduction of iron in individual aerosol particles [PC-017]**
Pablo Corral Arroyo, ETH Zurich
G. David, P. A. Alpert, E. A. Parmentier, M. Ammann, R. Signorell*
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- 14:30 **Spin-labeled nanobodies as conformation reporters of membrane proteins in cells [PC-021]**
Enrica Bordignon, University of Geneva
L. Galazzo, G. Meier, D. Januliene, A. Moeller, M. A. Seeger
- 15:00 **Molecular light-upconversion: when excited state absorption (ESA) overcomes energy transfer upconversion (ETU) in Cr(III)/Er(III) complexes [PC-023]**
Ines Taarit, University of Geneva
B. Galesorkhi, C. Piguet*
- 15:15 **Optical spectroscopy of crystal nucleation one nucleus at a time [PC-024]**
Oscar Urquidi, University of Geneva
J. Brazard, N. LeMessurier, L. Simine, T. Adachi
- 15:30 **First *in situ* THz measurements on organic electrochemical transistors: New perspectives from the microscale [PC-025]**
Gonzague Rebetz, University of Bern
O. Bardagot, J. Réhault, N. Banerji*
- 15:45 **Ultrafast process(es) in strongly confined perovskite nanocrystals [PC-026]**
Etienne Socie, EPFL Lausanne
J. Moser*
- 16:00 **Directed evolution of nanosensors for the detection of mycotoxins [PC-027]**
Benjamin Lambert, EPFL Lausanne
A. Taheri, S. Wu, A. J. Gillen, A. A. Boghossian*

Polymers, Colloids & Interfaces [PI]

Session Endowment: EMS Chemie

Chairs: Prof. Esther Amstad, EPFL Lausanne
Dr. Kuljeet Kaur, EPFL Lausanne

- 11:00 **Colour with a twist: from cellulose to large scale production of interference pigments [PI-011]**
Silvia Vignolini, Cambridge University
- 11:30 **Loop structures for strain sensing in elastomers [PI-013]**
Hanna Traeger, Adolphe Merkle Institute, Fribourg
Y. Sagara, J. Clough, D. Kiebal, J. Berrocal, S. Schrettl*, C. Weder*
- 11:45 **Thermoplastic Toughening of Semiaromatic Polyamides Using Amine-terminated Polyethylene [PI-014]**
Michael Giffin, EPFL Lausanne
C. J. Plummer, H. Frauenrath*
- 12:00 **Tuning Dispersity by Photoinduced Atom Transfer Radical Polymerisation: Monomodal Distributions with ppm Copper Concentration. [PI-015]**
Richard Whitfield, ETH Zurich
K. Parkatzidis, M. Rolland, N. P. Truong, A. Anastasaki*
- 12:15 **Amphiphilic Polymer Conetworks – Wearable and High Energy Transfer Rate Luminescent Solar Concentrators [PI-016]**
Chieh-Szu Huang, Empa
K. Jakubowski, S. Ulrich, S. Yakunin, L. F. Boesel*, M. V. Kovalenko*
- 12:30 **Bacteria-Induced Mineralization of 3D Printed Hydrogel Structures [PI-017]**
Matteo Hirsch, EPFL Lausanne
S. Ait Said, A. Clarà Saracho, E. Amstad*
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- 14:30 **tbd [PI-021]**
Botho Hoffmann, EMS Chemie
- 15:00 **Programming of Self-Assembly in Time with Chemical Clocks [PI-023]**
Guido Panzarasa, ETH Zurich
N. Lentz*
- 15:15 **Understanding the role of monomer-monomer interactions in the formation of semi-crystalline surface patterns from trimeric DNA macromolecules [PI-024]**
Vincenzo Caroprese, EPFL Lausanne
C. Tekin, V. Cencen, G. Fantner*, M. M. C. Bastings*
- 15:30 **Self-Assembly of Polymeric Nanocapsules towards Multi-Functional Supracapsules [PI-025]**
Minghan Hu, ETH Zurich
N. Reichholf, L. A. Frances, S. N. Ramakrishna, Y. Xia, X. Cao, S. Ma, A. J. deMello, L. Isa*, M. Hu*
- 15:45 **Physical characterization of virus-like particles carrying B cell epitopes for surface glycoprotein of SARS-CoV-2 virus [PI-026]**
Milad Radiom, ETH Zurich
Y. Nikolova, S. Peret, T. Keys, V. Bueno, P. Nylund*, E. Slack*
- 16:00 **Non-Classical Reaction Behavior of Complex Molecular Systems Based on Coupled Assembly Processes [PI-027]**
Tobias Schnitzer, Eindhoven University of Technology
M. F. Mabesoone, S. A. Jansen, G. Vantomme, B. Meijer*

VIRTUAL POSTER SESSIONS (SHORT VIDEOS)**Poster Presentation Title [Code]**

First line = Presenting Author, Affiliation

Second line = Co-authors

* Research Head(s)

Analytical Sciences [AS]**Virtual Poster Session****Cryogenic infrared spectral decomposition for glycan isomer identification [AS-101]**

Ali Abikhodr, EPFL Lausanne

V. Yatsyna, T. R. Rizzo*

Identification of positional isomers of N-linked glycans: A cryogenic IR spectroscopy database approach [AS-102]

Priyanka Bansal, EPFL Lausanne

A. Ben Faleh, P. Rzepka, T. R. Rizzo*

Aerosols in Low Dispersion Laser Ablation Inductively Coupled Plasma Mass Spectrometry [AS-103]

Pascal Becker, ETH Zurich

V. Wyss*

Rapid detection of volatile organic molecules with widely electrically tuneable quantum-cascade lasers [AS-104]

Raphael Brechbühler, Empa

P. Scheidegger, H. Looser, A. Kupferschmid, L. Emmenegger, B. Tuzson

Cyclodextrins in Mass Spectrometry [AS-105]

Pia Bruni, University of Bern

S. Schürch*

CERN-IRA Competence Centre for Internal Dosimetry and Incorporation Measurements of Radionuclides [AS-107]

Ruslan Cusnir, University Hospital of Lausanne

S. Medici, P. Froidevaux, P. Carbonez, M. Straub*

In situ isotope dating using LMS-GT – a high mass resolution laser ablation ionization mass spectrometer [AS-108]

Coenraad de Koning, University of Bern

A. Riedo, V. Grimaudo, P. Keresztes Schmidt, N. Boeren, S. Gruchola, M. Tulej, R. Lukmanov, N. F. Ligterink, P. Wurz*

Influence of linker length and dye flexibility on Förster resonance energy transfer in the gas phase [AS-109]

Jonas Metternich, ETH Zurich

P. Tiwari, R. Zenobi*

Identification of Stable Protein Standards for Ion Mobility Analysis [AS-110]

Julian Harrison, ETH Zurich

R. Zenobi

Compressive signal collection for dynamic X-ray Absorption Spectroscopy [AS-111]

Yousuf Hemani, Empa

D. Bleiner, D. Bleiner*

In-situ characterization of gold nanoparticles colloidal stability in biological environments [AS-112]

Neda Iranpour, Empa

M. Liebi, Q. Ong, P. Wick, A. Neels*

Integration of a microchip laser system into a laser desorption/ablation mass spectrometer built for space applications [AS-113]

Peter Keresztes Schmidt, University of Bern
N. Boeren, M. Tulej, P. Wurz*, A. Riedo*

Synthesis and characterization of new single-chain C18-chloropaffin materials by LC-Orbitrap-MS [AS-114]

Marco Knobloch, Empa
J. Sprengel, U. Stalder, J. Hutter, F. Mathis, S. Kern, W. Vetter, L. Bigler, N.V. Heeb, D. Bleiner*

High-throughput Single-cell Mass Spectrometry Reveals Abnormal Lipid Metabolism in Pancreatic Ductal Adenocarcinoma [AS-115]

Qinlei Liu, ETH Zurich
W. Ge, T. Wang, J. Lan, S. Martínez-Jarquín, C. Wolfrum, M. Stoffel, R. Zenobi*

Analysis of mycotoxins by swab spray ionization mass spectrometry [AS-116]

Lara Maeder, University of Bern
T. Muggli, S. Schürch*

Paper sampling for trace compounds with Ambient Ionization Mass Spectrometry [AS-117]

Sandra Martínez-Jarquín, ETH Zurich
A. I. Begley, Y. Lai, G. L. Bartolomeo, P. Adam, R. Zenobi*

Depth-Profiling Analysis at the Micro-Nano Scale with Soft X-rays and Chemometrical Postprocessing [AS-118]

Claudia Masucci, University of Zurich/ Empa
D. Bleiner*

Construction and optimization of a swab spray ion source [AS-119]

Thomas Muggli, University of Bern
L. Maeder, S. Schürch*

Quantum cascade laser absorption spectroscopy of clumped $^{12}\text{C}^{18}\text{O}^{18}\text{O}$ [AS-120]

Akshay Nataraj, ETH Zurich
M. Gianella, I. Prokhorov, B. Tuzson, J. Faist, L. Emmenegger*

Competitive and cheaper: LA-ICP-MS using a nitrogen plasma source [AS-121]

Christoph Neff, ETH Zurich
P. Becker, B. Hattendorf, V. Wyss*

Tip-enhanced Raman Spectroscopy on Two-Dimensional Polymers [AS-122]

Timo Niepel, ETH Zurich
W. Wang, A. D. Schlüter, R. Zenobi*

Hyperspectral imaging of supported lipid monolayers using Tip-Enhanced Raman Spectroscopy (TERS) [AS-123]

Yashashwa Pandey, ETH Zurich
N. Kumar, G. Goubert, R. Zenobi*

Optical clumped isotope $\Delta^{13}\text{CH}_3\text{D}$ and $\Delta^{12}\text{CH}_2\text{D}_2$ analyses open up new geochemical frontiers [AS-124]

Ivan Prokhorov, Empa
B. Tuzson, L. Emmenegger, S. M. Bernasconi, J. Mohn

Laser-Induced XUV Spectroscopy (LIXS) for High-Precision Lithium Analysis of Energy Materials [AS-125]

Di Qu, Empa
D. Bleiner*

Measurements of atmospheric nitrogen dioxide and nitric acid using Quantum Cascade Absorption Spectroscopy. [AS-126]

Nicolas Sobanski, Empa
B. Tuzson, P. Scheidegger, H. Looser, A. Kupferschmid, M. Iturrate, B. Schwarzenbach, C. Hüglin, L. Emmenegger*

An Optical Polyion Nanosensor based on Internal Hydrophobicity/Hydrophilicity Solvatochromism for Heparin Detection in Plasma [AS-127]

Yoshiki Soda, University of Geneva
K. J. Robinson, R. Nussbaum, E. Bakker*

Asthma biomarker discovery in exhaled breath by secondary electrospray ionization mass spectrometry [AS-128]

Bettina Streckenbach, ETH Zurich
R. Weber, S. Micic, T. Bruderer, D. Inchi, L. Welti, N. Perkins, R. Zenobi*, A. Moeller*

Can vibrational spectroscopy finally find its place in the world of analytical mass spectrometry? [AS-129]

Stephan Warnke, EPFL Lausanne
A. Ben Faleh, P. Bansal, T. R. Rizzo*

On-Line Breath Analysis using Secondary Electrospray Ionization MS upon a Nutritional Challenge Test [AS-130]

Cedric Wüthrich, ETH Zurich
M. de Figueiredo, S. Giannoukos*, R. Zenobi*

Symmetric solid-contact potentiometric system [AS-131]

Elena Zdrachek, University of Geneva
T. Forrest, E. Bakker*

**Catalysis Sciences & Engineering [CE]
Virtual Poster Session****Unravelling the aging phenomena of Diesel oxidation catalysts [CE-101]**

Miren Agote-Aran, Paul Scherrer Institute, Villigen
M. Elsener, C. M. Schilling, F. W. Schütze, M. Sridhar, E. Katsaounis, O. Kröcher, D. Ferri*

Ga⁰-Cu ratio as the main descriptor of the catalytic activity of Ga promoted Cu nanoparticle based catalysts for CO₂ hydrogenation to Methanol [CE-102]

Jan Alfke, Paul Scherrer Institute, Villigen
M. Tejada Serrano, T. Z. Gani, C. Copéret*, O. Safonova*

Electrochemical Reduction of CO₂ on Au Electrocatalysts Under Commercially Relevant Condition [CE-103]

Shima Alinejad, University of Bern
J. Quinson, Y. Li, S. Reichenberger, M. Arenz*

The structural and kinetic signatures of the copper sites in mordenite for methane oxidation to methanol [CE-104]

Mikalai Artsiusheuski, ETH Zurich
D. Klose, G. Jeschke, J. A. van Bokhoven, V. Sushkevich*

Ultrahigh permeance metal coated porous graphene membranes with tunable gas selectivities [CE-105]

Timur Ashirov, University of Fribourg
A. Coskun*

Correlating Lewis Acid Activity to Extra-Framework Aluminum in Zeolite Y Introduced by Ion-Exchange [CE-106]

Syeda Batool, ETH Zurich
V. Sushkevich, J. A. van Bokhoven*

Activity and initiation of silica-supported Mo olefin metathesis catalysts in the liquid phase [CE-107]

Zachariah Berkson, ETH Zurich
G. Price, G. Sunley, C. Copéret*

Solid catalysts aerobically catalyze the conversion of methane to methyl derivatives in high yields under improved conditions [CE-108]

Andrea Blankenship, ETH Zurich
M. Ravi, J. A. van Bokhoven*

Testing supported IrO_x and IrRuO_x nanocatalysts for the acidic oxygen evolution reaction in a novel gas diffusion electrode setup [CE-109]

Aline Bornet, University of Bern
E. Berner, J. Quinson, J. Schröder, M. Arenz*

Highly Selective Pd-P-MOF-catalyzed mild Suzuki Reactions [CE-110]

Daniele Cartagenova, Paul Scherrer Institute, Villigen
S. Bachmann, K. Püntener, M. Scalone, M. A. Newton, J. A. van Bokhoven, M. Ranocchiari*

Mapping the hydrocarbon pool formation and coke generation in C₁ coupling over zeolite catalysts [CE-111]

Alessia Cesarini, ETH Zurich
G. Zichittella, P. Hemberger, M. Agrachev, A. Bodi, G. Jeschke, S. Mitchell, J. Pérez-Ramírez*

Understanding and fine-tuning of lignin fast pyrolysis towards phenolics and aromatics [CE-112]

Lunhan Chen, ETH Zurich
A. Puente-Urbina, Z. Pan, R. Haaring, P. Hemberger, J. A. van Bokhoven*

In-situ SEM investigation on the active state of nickel catalyst in dry reforming of methane [CE-113]

Claudiu Colbea, ETH Zurich
M. G. Willinger, J. A. van Bokhoven*

Pt-based Nanocomposite Catalysts for the Oxygen Reduction Reaction in Rotating Disk Electrode and Gas Diffusion Electrode measurements [CE-114]

Jia Du, University of Bern
J. Quinson, A. Zana, M. Arenz*

SynFuel: Development of a new synthetic pathway for the production of renewable jet-fuels from methanol [CE-115]

Florent Dubray, Paul Scherrer Institute, Villigen
V. Paunović, M. Ranocchiari, J. A. van Bokhoven*

Scalable two-step annealing method for preparing ultra-high-density single-atom catalyst libraries [CE-116]

Dario Faust Akl, ETH Zurich
S. Mitchell, X. Hai, J. Pérez-Ramírez*, J. Lu*

SynFuels - an ETH initiative for the production of synthetic jet fuels - Thermochemical routes [CE-117]

Davide Ferri, Paul Scherrer Institute, Villigen
J. A. van Bokhoven, M. Nachtegaal, T. Schildhauer, M. Ranocchiari, F. Vogel, D. Ferri*

Following the sintering behavior of Platinum by in Situ STEM aided by artificial intelligence [CE-118]

Hannes Frey, ETH Zurich
A. Beck, M. G. Willinger*, J. A. van Bokhoven*

Adsorption Effects of Zn-MOF-74 in Cobalt-Catalyzed Hydroformylation [CE-119]

Patrick Gäumann, Paul Scherrer Institute, Villigen
D. Ongari, B. Smit, J. A. van Bokhoven, M. Ranocchiari*

Controlled formation of dimers and spatially isolated atoms in Au-Ru single-atom catalysts via carbon-host functionalization [CE-120]

Vera Giulimondi, ETH Zurich
S. K. Kaiser, A. J. Martín, S. Buchele, F. Krumeich, A. H. Clark, J. Pérez-Ramírez*

Selective conversion of polypropylene into motor oil on carbon-supported platinum catalysts [CE-121]

Shibashish Jaydev, ETH Zurich
A. J. Martín, J. Pérez-Ramírez*

Selective monografting of Al(III) sites on the surface of silica [CE-122]

Maciej Korzynski, ETH Zurich
Z. J. Berkson, C. Copéret*

¹⁵N NMR Chemical Shift Tensor as Acidity Descriptor for Al-O(H)-Al sites in Molecular Aluminosilicate Models and Link to Reactivity [CE-123]

Lukas Lätsch, ETH Zurich
F. Beckmann, K. S. Lokare, C. Copéret*, C. Limberg*

Structure-activity evolution of platinum species supported on ceria exposed to different reaction environments [CE-124]

Xiansheng Li, Paul Scherrer Institute, Villigen
J. A. van Bokhoven, L. Artiglia

Oxidative Dehydrogenation of Ethane with in situ Oxygen Production via Chemical Looping with Oxygen Uncoupling [CE-125]

Giancarlo Luongo, ETH Zurich
F. Donat, C. Müller*

Planetary footprints of low-carbon ammonia [CE-126]

Antonio Martín, ETH Zurich
S. C. D'Angelo, V. Tulus, J. Pérez-Ramírez*, G. Guillén-Gosálbez*

Copper Nanoparticles under CO₂ Hydrogenation Conditions - Shape and Surface Morphology from First Principles and Variation due to Promoter Inclusion [CE-127]

Andreas Müller, ETH Zurich
A. Comas-Vives, C. Copéret*

Reversible phase transitions in novel Ce-substituted perovskite oxide composites for solar thermochemical CO₂ redox splitting [CE-128]

J. Madhusudhan Naik, University of Zurich
C. Ritter, B. Bulfin, A. Steinfeld, R. Erni, C. Cadoux*

Hydrogen spillover in hydrogenation catalysts by neutron imaging [CE-129]

Marin Nikolic, Empa
A. Borgschulte, E. Billeter, O. Sambalova, T. Pavel

Investigation of HCN formation from formaldehyde during the selective catalytic reduction of NO_x with NH₃ over V₂O₅/WO₃-TiO₂ [CE-130]

Rob Jeremiah Nuguid, Paul Scherrer Institute, Villigen
M. Elsener, D. Ferri*, O. Kröcher*

Potassium Magnesiata Catalysed Hydrophosphinylation of Styrenes [CE-131]

Andrew Platten, University of Bern
A. M. Borys, E. Hevia*

Palladium single-atoms supported on nitrogen doped carbon for Sonogashira cross-coupling [CE-132]

Dario Poier, ETH Zurich
D. Faust Akl, S. Mitchell, R. Marti*, J. Pérez-Ramírez*

Molecular Transformer-aided Biocatalysed Synthesis Planning [CE-133]

Daniel Probst, IBM Research Europe
M. Manica, Y. G. Nana Teukam, A. Castrogiovanni, F. Paratore, T. Laino*

Mechanistic insights on the conversion of methane under non-oxidative conditions over iron-modified silica [CE-134]

Allen Puente-Urbina, ETH Zurich
Z. Pan, V. Paunovič, P. Šot, P. Hemberger, J. A. van Bokhoven*

Exploiting resonant X-ray powder diffraction at the Al K edge to locate aluminum in zeolite frameworks [CE-135]

Przemyslaw Rzepka, EPFL Lausanne
A. B. Pinar, A. J. Knorpp, L. B. McCusker, C. Baerlocher, T. Huthwelker, J. A. van Bokhoven*, L. B. McCusker*

Iron-associated active oxygen species are responsible for low-temperature catalytic activity of Pt-FeO_x/Al₂O₃ catalyst [CE-136]

Iliya Sadykov, Paul Scherrer Institute, Villigen
M. Zabilskiy, J. A. van Bokhoven, A. H. Clark, V. Sushkevich, F. Krumeich, M. Nachttegaal, O. Safonova*

Design of carbon supports for metal-catalyzed acetylene hydrochlorination [CE-137]

Ivan Surin, ETH Zurich
S. K. Kaiser, A. Amorós-Pérez, S. Buchele, F. Krumeich, A. H. Clark, M. C. Román-Martínez, M. A. Lillo-Ródenas, J. Pérez-Ramírez*

Gold supported on ceria as a superior catalyst for nitrous oxide production via direct ammonia oxidation [CE-138]

Ivan Surin, ETH Zurich
Z. Tang, A. Rasmussen, J. Pérez-Ramírez*

Hydrogen Dissociation Sites on Indium-Based ZrO₂-Supported Catalysts for Hydrogenation of CO₂ to Methanol [CE-139]

Athanasia Tsoukalou, ETH Zurich
A. Serykh, E. Willinger, A. Kierzkowska, P. Abdala, A. Fedorov*, C. R. Müller*

Toward reliable and accessible ammonia quantification in the electrocatalytic reduction of nitrogen [CE-140]

Florentine Veenstra, ETH Zurich
A. J. Martín, J. Lüthi, R. Verel, J. Pérez-Ramírez*

Catalytic activity of cobalt sulfide for alkene epoxidation [CE-141]

Vanessa Wyss, University of Basel
F. Dubray*

Elucidating the mechanism of oxidative dehydrogenation of ethanol over V₂O₅/TiO₂ by transient XAS [CE-142]

Anna Zabilska, Paul Scherrer Institute, Villigen
A. H. Clark, I. Wachs, M. Nachttegaal, O. Kröcher, O. Safonova*

Influence of preparation method on Pt/Al₂O₃ catalysts activity in the hydrogenation of nitrobenzene to aniline [CE-143]

Damin Zhang, University of Bern
M. Arenz*

Ultra-Thin Coordination Polymer Derivatives Towards Efficient Oxygen Generation [CE-144]

Yonggui Zhao, University of Zurich
C. Cadoux

Synthesis and catalytic activity of SOMC-derived Co nanoparticles [CE-145]

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

A unified understanding of indium oxide promotion by transition metals at the atomic scale [CE-146]

Tangsheng Zou, ETH Zurich
T. Pinheiro Araújo, P. Willi, R. García-Muelas, J. Morales-Vidal, O. Safonova, N. López, R. Grass, C. Mondelli, J. Pérez-Ramírez*

**Computational and Theoretical Chemistry [CC]
Virtual Poster Session****Instanton Theory Beyond Golden Rule: Three-state System [CC-101]**

Imaad Ansari, ETH Zurich
G. Trenins, E. R. Heller, J. O. Richardson*

Combining accuracy with linear-scaling efficiency: energies and nuclear gradients for a variational formulation of the Harris functional as correction to sub-system DFT [CC-102]

Fabian Belleflamme, University of Zurich
A. Hehn, J. Hutter*, M. Iannuzzi*

Diffusio-osmotic transport of hydrophobic solutes and slippage opacity of two-dimensional materials [CC-103]

Maria Bilichenko, University of Zurich
G. Tocci, J. Hutter, M. Iannuzzi*

Optimal tunneling pathways for proton-coupled electron transfer reactions [CC-104]

Martin Bircher, ETH Zurich
E. R. Heller, J. O. Richardson*

Solvation Free Energies from Subsystem Density Functional Theory with Sampling [CC-105]

Paul Türtcher, ETH Zurich
M. Bensberg, J. P. Unsleber, J. Neugebauer*, M. Reiher*

Rapid screening of nanopores in graphene for light hydrocarbons separation [CC-106]

Luc Bondaz, EPFL Lausanne

Unprecedented Water-Assisted Chemical Route Towards the Oxygen Evolution Reaction at the Hydrated (110) Ruthenium Oxide Surface: heterogeneous catalysis via DFT-MD & metadynamics simulations [CC-107]

Fabrizio Creazzo, University of Zurich
S. Luber*

An implementation of Nuclear Velocity Perturbation Theory using a combined Gaussian and plane wave basis set [CC-108]

Edward Ditley, University of Zurich
S. Luber*

Chemical Concepts in Automated Reaction Network Exploration [CC-109]

Stephanie Grimmel, ETH Zurich
M. Reiher*

Fast prediction of correlation energies for Møller–Plesset perturbation theory: atomic contribution model and machine learning [CC-110]

Ruo Cheng Han, University of Zurich
S. Lubner*

Tailoring absorption and fluorescence spectra for nanoporous materials [CC-111]

Anna Hehn, University of Zurich
B. Sertcan, F. Belleflamme, S. Chulkov, M. Watkins, J. Hutter*

Predicting Enzymatic Reactions with a Molecular Transformer [CC-112]

David Kreutter, University of Bern
P. Schwaller, J. Reymond*

Evaluating Quantum Mechanical Tunnelling Splittings with Instanton Theory [CC-113]

Gabriel Laude, ETH Zurich
M. Fiechter, J. O. Richardson*

A novel quantum-classical approach to electronic nonlinear spectroscopy [CC-114]

Jonathan Mannouch, ETH Zurich
J. O. Richardson*

Tailored Coupled Cluster Theory in Varying Correlation Regimes [CC-115]

Maximilian Mörchen, ETH Zurich
L. Freitag, M. Reiher*

Real-Time Haptic Chemistry: Dive Hands-First into the Molecular World [CC-116]

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

Using GAFF topologies and RE-EDS to calculate relative hydration free energies in GROMOS [CC-117]

Salomé Rieder, ETH Zurich
B. Ries, C. Champion, P. H. Hünenberger, S. Riniker*

Quantum-DFT Embedding Algorithm for Electronic Structure Calculations [CC-118]

Max Rossmannek, IBM Research Europe
P. Barkoutsos, P. Ollitrault, V. Weber, V. Rybkin, J. Hutter*, I. Tavernelli*

Time-reversible and norm-preserving implicit split-operator algorithms for the nonlinear time-dependent Schrödinger equation [CC-119]

Julien Roulet, EPFL Lausanne
J. Vaníček*

Simulation of quantum entanglement with classical trajectories [CC-120]

Johan Runeson, ETH Zurich
J. O. Richardson*

Low-data regime yield predictions with uncertainty estimation using deep learning approaches [CC-121]

Philippe Schwaller, IBM Research Europe
A. C. Vaucher, T. Laino*, J. L. Reymond*

A computational study of kinetic trapping of noble gases in metal organic frameworks [CC-122]

Beliz Sertcan, University of Zurich
A. Hehn, H. Bunzen, D. Volkmer, M. Iannuzzi, J. Hutter*

Accessing the Conformational Space of Cyclosporin A in Chloroform Using RDCs as Tensorial Constraints [CC-123]

Thomas Stadelmann, ETH Zurich
M. Ebert*, S. Riniker*

How to Accelerate Double-Hybrid Calculations to Determine Cohesive Energies in Metal Organic Framework [CC-124]

Frederick Stein, University of Zurich
J. Hutter*

Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis [CC-125]

Miguel Steiner, ETH Zurich
M. Reiher*

Nonadiabatic Quantum Transition State Theory Instanton Rates beyond Golden Rule [CC-126]

Georgijs Trenins, ETH Zurich
J. O. Richardson*

Chemoton 2.0: Automated Exploration of Reaction Networks [CC-127]

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

Inferring missing molecules in incomplete chemical equations [CC-128]

Alain Vaucher, IBM Research Europe
P. Schwaller, A. Toniato, T. Laino*

To tunnel or not to tunnel - in the aqueous ferrous-ferric system [CC-129]

Rhiannon Zarotiadis, ETH Zurich
W. Fang, J. O. Richardson*

**Chemistry and the Environment [EV]
Virtual Poster Session****Seasonal aerosol acidity and liquid water content: impact on aerosol concentration and nitrogen deposition fluxes in Toronto [EV-101]**

Andrea Arangio, EPFL Lausanne
P. Shahpoury, E. Dabek-Zlotorzynska, A. Nenes

Influence of Transition Metals on Particle-bound Reactive Oxygen Species and the Oxidative Potential of Secondary Organic Aerosol Particles [EV-102]

Alexandre Barth, University of Basel
B. Uttinger, S. J. Campbell, M. Kalberer*

One-step extraction of multifunctional lignins from lignocellulosic biomass [EV-103]

Stefania Bertella, EPFL Lausanne
J. S. Luterbacher*

Detection and Characterisation of Criegee Intermediates in Secondary Organic Aerosol Particles [EV-104]

Steven Campbell, University of Basel
K. Wolfer, P. J. Gallimore, C. Giorio, D. Häussinger, M. Kalberer*

Catalyst-membrane synergy as a means of improving process intensity and catalyst or metal recovery. [EV-105]

Sergio Cuesta-Galisteo, University of Zurich
T. Al Chami Al Bayrakdar, A. Buekenhout, F. Nahra, S. P. Nolan

Surface bound molybdenum for the electrochemical detection of phosphate [EV-106]

Polyxeni Damala, University of Geneva
T. Cherubini, E. Bakker*

Bimetallic Palladium-Gallium catalysts for the hydrogenation of CO₂ to Methanol [EV-107]

Scott Docherty, ETH Zurich
C. Copéret*

Submersible Probe with In-line Calibration and Symmetrical Reference Element for Long-term Continuous Measurements [EV-108]

Tara Forrest, University of Geneva
T. Cherubini, S. Jeanneret, E. Zdrachek, P. Damala, E. Bakker*

Tetraaza[14]annulene-Based Covalent Organic Frameworks: An Intriguing Class of Catalytically Active Porous Materials [EV-109]

Patrick Fritz, University of Fribourg
A. Coskun*

Autonomous in situ voltammetric monitoring of inorganic arsenic speciation [EV-110]

Tanguy Gressard, University of Geneva
N. Layglon, M. Tercier-Waeber*

Ensuring healthy babies through non-target screening of disposable baby diapers [EV-111]

Griet Jacobs, VITO

Chemical Mechanism of Microbial Metal Reduction [EV-112]

Maksym Karamash, University of Fribourg
B. Giese*, K. M. Fromm*

Engineering extracellular electron transfer in Escherichia coli for microbial electrochemical systems [EV-113]

Mohammed Mouhib, EPFL Lausanne
M. Reggente, L. Li, A. A. Boghossian*

Predicting pesticide biotransformation products and half-lives in soil and sediment [EV-114]

Mohammed Mouhib, EPFL Lausanne
D. Latino, M. Salz, K. Fenner*

Bioengineered photosynthetic bacteria for enhanced electrogenic capabilities [EV-115]

Melania Reggente, EPFL Lausanne
M. Mouhib, A. A. Boghossian

Carbon nanotube uptake in photosynthetic bacteria enhanced bioelectricity generation in living photovoltaics [EV-116]

Melania Reggente, EPFL Lausanne
A. Antonucci, C. Roullier, A. J. Gillen, N. Schürgers, V. Zubkovs, M. Mouhib, B. Lambert, A. A. Boghossian

Fluorescent pH-Sensitive Wood Membranes [EV-117]

Maximilian Ritter, ETH Zurich
G. Panzarasa, N. Lentz*

Estimation of Swiss Halocarbon Emissions Using Regional Atmospheric Measurements [EV-118]

Dominique Rust, Empa
I. Katharopoulos, M. K. Vollmer, S. Henne, M. Hill, L. Emmenegger, R. Zenobi, S. Reimann*

Co/Ni-Polyoxotungstates as photocatalysts and precursors for electrocatalytic water oxidation [EV-119]

Giann Wiprächtiger, University of Zurich
R. Güttinger, O. Blacque, C. Cadoux*

Stable Solid Electrolyte Interphase Formation Induced by Monoquat-Based Anchoring in Lithium Metal Batteries [EV-120]

Tianhong Zhou, University of Fribourg
Y. Zhao, A. Coskun*

Inorganic Chemistry [IC] Virtual Poster Session

Targeted Design of Binuclear Copper Complexes for Efficient Electrocatalytic Water Oxidation [IC-101]

Devi Adiyeri Saseendran, University of Zurich
G. R. Patzke*

Structure Elucidation of Colloidal Perovskite Nanocrystals by Solution NMR [IC-102]

Marcel Aebli, ETH Zurich
N. Yazdani, F. Krieg, D. Guggisberg, C. Bernasconi, M. Marczak, M. V. Kovalenko*, V. Wood*

Sulfur-Transfers on Transition Metal Phosphide Surfaces [IC-103]

Nina Arnosti, University of Basel
F. Dubray*

Effect of missing-linker defects on crystalline stability of UiO-66 under different gaseous conditions [IC-104]

Muhammad Athar, Paul Scherrer Institute, Villigen
M. Ranocchiaro*, J. A. van Bokhoven*

Reactivity of a 5-Coordinated Unsaturated Pya ruthenium(II) Complex [IC-105]

Alicia Beaufils, University of Bern
P. Melle, M. Albrecht*

Interaction of small molecules with ⁹⁹Tc pincer-type complexes [IC-106]

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

The Structurally Diverse Anionic Pathway in the Nickel-Catalysed Cross Coupling of Aryl Ethers [IC-107]

Andryj Borys, University of Bern
A. M. Borys*, E. Hevia*

Crystal and Morphology Engineering of Poly (triazine imide) for Application in Molecular Separation [IC-108]

Heng-Yu Chi, EPFL Lausanne
K. Agrawal

Size and Composition Controlled Intermetallic Nanocrystals via Amalgamation Seeded Growth [IC-109]

Jasper Clarysse, ETH Zurich
A. Moser, O. Yarema, V. Wood*, M. Yarema*

Role of the Apparently Non-Interacting Substrate in Dioxygen Activation at Rieske Dioxygenases [IC-110]

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

Spectral Signatures of Ga Species Enabled by ^{71}Ga Nuclear Magnetic Resonance and $^{69}\text{Ga}/^{71}\text{Ga}$ Nuclear Quadrupole Resonance Spectroscopies [IC-111]

Scott Docherty, ETH Zurich
L. Völker, A. V. Yakimov, C. Copéret*, R. Verel*

Development of an electrochemical method to separate radioisotopes of cobalt and nickel [IC-112]

Paul Duthéil, Paul Scherrer Institute, Villigen
M. Heule, P. Steinegger

Rigidifying Bis(Benzimidazole)Pyridine Scaffolds: the Key to Improve Stability in Linear Lanthanidopolymers [IC-113]

Soroush Naseri, University of Geneva
H. Nozary, L. Guénée, C. Besnard, C. Piguet*

Competitive $\text{Csp}^2\text{-H}$ versus $\text{Csp}^3\text{-H}$ activation from Ph-PYA based Pt(IV) complexes [IC-114]

Albert Farre, University of Bern
M. Albrecht*

Cyclotron production and radiochemical purification of the radiolanthanide terbium-155 for potential application in nuclear medicine [IC-115]

Chiara Favaretto, Paul Scherrer Institute, Villigen
Z. Talip, F. Borgna, P. V. Grundler, H. Zhang, C. Müller, R. Schibli, N. P. van der Meulen*

Stabilizing CsPbBr_3 Nanocrystals: AlO_x Gel Capping from a Non-Hydrolytic Sol-Gel Reaction [IC-116]

Dominic Guggisberg, ETH Zurich
S. Yakunin, C. Zhu, G. Rainò, M. V. Kovalenko*

Interdependence of structural and compositional parameters on up-converting hafnia nanoparticles [IC-117]

Xavier Guichard, ETH Zurich
A. Lauria*

The Bi^{3+} Lone Pair Effect in $(\text{H}_3\text{O})\text{Bi}(\text{SO}_4)_2$, $\text{Bi}(\text{HSO}_4)_3$ and $\text{Bi}_2(\text{SO}_4)_3$ [IC-118]

Matthias Hämmer, Universität Augsburg
J. Brgoch, P. Netzsch, H. A. Höpfe*

Mechanistic Study on Thermally Induced Lattice Stiffening of ZIF-8 [IC-119]

Jian Hao, EPFL Lausanne
K. Agrawal*

Angstrom-scale etching and functionalization of porous graphene lattice [IC-120]

Kuang-Jung Hsu, EPFL Lausanne
K. Agrawal*

Superheavy Element Chemistry and the Residual Gas Effects on the Chromatographic Yield of Homologs Hg and At [IC-121]

Paul Ionescu, University of Bern
P. Steinegger, R. Eichler, R. Dressler, N. M. Chiera, A. Türlér*

Stepwise reduction of dinitrogen to nitride by a uranium-potassium complex [IC-122]

Nadir Jori, EPFL Lausanne
L. Barluzzi, I. Douair, L. Maron, I. Zivkovic, L. Xu, M. Mazzanti*

Exploring the alkali metal and alkoxide effects in Mg-Br exchange reactions using mixed alkyl/alkoxy alkali metal magnesiates. [IC-123]

Neil Judge, University of Bern
L. J. Bole, E. Hevia*

Macrocyclic Ligands: From Synthesis Towards On-Surface Topology, and their Candidacy as Synthons for Interlaced Structures [IC-124]

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

Self Supporting Polymers of Ir-NHC Complexes [IC-125]

Pascal Knörr, University of Bern
M. Albrecht*

 $\text{CeZn}_{2-8}\text{Ge}_2$: New Zn-deficient CaBe_2Ge_2 -Type Phase with Rare Ce-based Ferromagnetism and Large Magnetoresistance [IC-126]

Robin Lefèvre, University of Zurich
F. O. von Rohr, F. O. von Rohr*

Cooperative bis(pyridylidene-amine) ligands for efficient palladium catalyzed formic acid dehydrogenation [IC-127]

Nicolas Lentz, University of Bern
M. Albrecht*

Direct Co-H exchange reactions of Fluoroarenes mediated by a mixed-metal Na/Co(II) base [IC-128]

Alessandra Logallo, University of Bern
E. Hevia*

Low-Valent Molybdenum Complexes Supported by Redox-Active β -Diketonate Ligands [IC-129]

Fabio Masero, ETH Zurich
M. Wörle, D. F. Abbott, V. Mougel*

Tandem Mn-I exchange and homocoupling processes mediated by Li/Mn cooperativity [IC-130]

Pasquale Mastropiero, University of Bern
M. Uzelac*, E. Hevia*

Deciphering Coordination Sites Affinity in Linear Multi Site Metallopolymers [IC-131]

Mohsen Mirzakhani, University of Geneva
H. Nozary, C. Besnard, C. Besnard, C. Piguet*

Cooperative Generation of Metal hydride via Bioinspired Proton Coupled Electron Mediator: Application to CO_2 reduction [IC-132]

Victor Mougel*, ETH Zurich

To Low-Valency and Back: Initiation Pathway for High-Valent Molybdenum-Oxo Species in Olefin Metathesis through molecular model systems [IC-133]

Darryl Nater, ETH Zurich
C. Kaul, N. Kaeffer, C. Copéret*

The development of new luminescent MOFs for molecular detection [IC-134]

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

Electronically asymmetric pyridyl-pyridylidene amide ligands for palladium-catalyzed copolymerization of alkenes and polar co-monomers [IC-135]

Esaïe Reusser, University of Bern
M. Albrecht*

Competitive etching and growth of graphene nanopores for molecular sieving [IC-136]

Mojtaba Rezaei, EPFL Lausanne
K. Agrawal*

A simple cerium-based chemosensor for selective fluorescence phosphate detection in aqueous media [IC-137]

Thibaud Rossel, University of Neuchâtel
B. Therrien, M. Mischler, K. Engel, G. Di Lullo, V. Picard, T. Rossel*

Characterization of the SINQ gas-jet facility as a source for fission products from ²³⁵U [IC-139]

Georg Tiebel, Paul Scherrer Institute, Villigen
P. Dutheil, J. M. Wilson, R. Dressler, R. Eichler, D. P. Herrmann, P. Steinegger*

Bottom-up synthesis of films hosting atom-thick molecular-sieving apertures [IC-140]

Cédric Van Goethem, EPFL Lausanne
L. F. Villalobos, K. Agrawal*

Radiochemical separation and purification of non-carrier-added silicon-32 for an accurate half-life redetermination [IC-141]

Mario Veicht, PSI, EPFL Lausanne
I. Mihalcea, Đ. Cvjetinovic, A. Pautz, D. Schumann*

Planar or Buckled? - Structure-Property Relationships in Superconductors with Honeycomb Layers [IC-142]

Dorota Walicka, University of Zurich
O. Blacque, F. O. von Rohr*

Isothermal gas adsorption chromatography of different thallium species for further investigations of nihonium [IC-143]

Jennifer Wilson, Paul Scherrer Institute, Villigen
N. V. Aksenov, S. N. Dmitriev, R. Eichler, B. Gall, N. S. Gustova, D. P. Herrmann, Y. A. Popov, A. I. Svirikhin, P. Steinegger*

Evaporation of radionuclides from heavy-liquid-metal-cooled reactors [IC-144]

Ivan Zivadinovic, ETH Zurich
P. Steinegger, J. Neuhausen*

**Medicinal Chemistry & Chemical Biology [MC]
Virtual Poster Session****Cooperativity of nitrogenase in biological nitrogen fixation [MC-101]**

Cécile Cadoux, University of Geneva
D. Ratcliff, L. Di Luzio, I. Tsakoumagkos, W. Gu, S. Hoogendoorn, R. D. Milton*

The Antimicrobial Activity of Peptide Dendrimers and Polymyxin B Increases Sharply Above pH 7.4 [MC-102]

Xingguang Cai, University of Bern
S. Javor, J. Reymond*

Restoring HIF-2 α Degradation in Clear Cell Renal Cell Carcinoma through PROTAC Technology [MC-103]

Carlotta Cecchini, University of Geneva
F. Costanzo, M. Héritier, S. Tardy, J. Theurillat, L. Scapozza*

Optimization of Covalent Chemical Probes [MC-104]

Martina De Pascale, University of Basel
C. Borsari, E. Keles, J. McPhail, A. Schäfer, R. Sriramaratnam, M. Gstaiger, J. Burke, M. Wymann

Novel Synthetic Strategies Enable the Efficient Development of Folate Conjugates for Radiotheragnostic Application [MC-105]

Luisa Deberle, Paul Scherrer Institute, Villigen
A. E. Becker, R. Schibli*, C. Müller*

An immunomodulatory Peptide Dendrimer Inspired from Glatiramer Acetate [MC-106]

Dina Erzina, University of Bern
A. Capecchi, S. Javor, J. Reymond*

Off-target profiling of Janus Kinase (JAK) inhibitors in rheumatoid arthritis: A computer-based approach for drug safety studies and repurposing [MC-107]

Maria Faquetti, ETH Zurich
F. Grisoni, P. Schneider, G. Schneider*, A. M. Burden*

Using chemical biology approaches to decipher chromatin ubiquitylation involving RNF168 [MC-108]

Pauline Franz, EPFL Lausanne
T. Pignard, B. Fierz*

Functionalized harmonic nanoparticles for cancer theranostics and multimodal imaging [MC-109]

Adrian Gheata, EPFL Lausanne
R. De Matos, J. Vuilleumier, G. Gaulier, G. Campargue, L. Bonacina, D. Staedler, D. Diviani, S. Gerber-Lemaire*

Cys-Cys and Cys-Lys stapling of unprotected peptides enabled by hypervalent iodine reagents [MC-110]

Elija Grinhagena, EPFL Lausanne
J. Ceballos, G. Sangouard, J. Waser*, C. Heinis*

Chemical Approach to Stabilise the Structure of Mitochondrial Carrier AGC2 (SLC25A13) [MC-111]

Philipp Grossenbacher, University of Bern
P. Damala, E. Kunji, M. Lochner*

Dual-Activatable Cell Tracker for Controlled and Prolonged Single Cell Labeling [MC-112]

Roman Günther, Zurich University of Applied Sciences ZHAW
E. A. Halabi, J. Arasa, V. Collado-Diaz, P. Rivera-Fuentes*, C. Halin*

Synthesis of potential protein-degrading drugs targeting the androgen-receptor in prostate cancer [MC-113]

Melanie Gut, University of Zurich
B. Dreier, A. Plückthun*, J. P. Holland*

A ratiometric sensor for live-cell imaging of dynamic glutathione concentration with subcellular precision [MC-114]

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

Systematic Tuning of Rhodamine Spirocyclization for Super-Resolution Microscopy [MC-115]

Nicolas Lardon, Max Planck Institute for Medical Research
L. Wang, A. Tschanz, P. Hoess, M. Tran, E. D'Este, J. Ries, K. Johnsson*

Rhenopaganib – an Organometallic Mimic of the Small Molecule Kinase Inhibitor Opaganib® [MC-116]

Raphael Lengacher, University of Zurich

O. Blacque, H. Braband, G. Gasser, R. Alberto*

A single-molecule multiplexed approach to study dCas9 nucleosomes invasion [MC-117]

Kristina Makasheva, EPFL Lausanne

L. Bryan, M. Jinek, B. Fierz*

Amino Acid Influence on Ag⁺ Binding Site in Model Peptides Inspired by the Silver Resistance Protein SilE [MC-118]

Florian Marquet, University of Fribourg

A. Bianchi, L. Babel, V. Chabert, K. M. Fromm*

Development of a New Synthetic Route for the Convenient Synthesis of Benzoxazinoid Compounds [MC-119]

Pierre Mateo, University of Bern

M. Erb*, C. A. Robert*

Development of stapled-peptide-based degraders of oncogenic chromatin factors [MC-120]

Grégoire Menoud, EPFL Lausanne

J. Waser, E. Grinhagena, B. Fierz*

Shaping the centromere – The role of CENP-B in modifying centromere chromatin [MC-121]

Harsh Nagpal, EPFL Lausanne

B. Fierz*

A robust ratiometric HaloTag reporter system for gene expression monitoring [MC-122]

Jade Nguyen, EPFL Lausanne

H. Lämmermann, P. Rivera-Fuentes*

Towards PROTAC-mediated degradation of CBP/EP300 [MC-123]

Leonardo Palaferri, University of Zurich

I. Cheng-Sánchez, K. Rollins, M. Kirillova, E. Laul, A. Müller, L. Wiedmer, A. Caflisch*, C. Nevado*

X-ray crystal structures of short mixed chirality α -helical antimicrobial peptides [MC-124]

Hippolyte Personne, University of Bern

S. Brunamonti, I. Di Bonaventura, T. Köhler, C. van Delden, A. Stocker, S. Javor, J. L. Reymond*

Structure-activity relationship study to find novel potent and selective adenosine A1 receptor agonists [MC-125]

Barbara Preti, University of Bern

A. Suchánková, K. Barkan, M. Leuenberger, M. Lochner*, G. Ladds*

Targeting RNA conformational ensemble of LMNA gene via Small Molecules against Hutchinson-Gilford Progeria Syndrome [MC-126]

Ece Sahi-Ilhan, University of Geneva

M. H. Bohnet, A. García-López, L. Scapozza*

Total Synthesis of FR252921 and Analogues: New Era in Immunosuppression? [MC-127]

Iakovos Saridakis, University of Vienna

M. Schupp, M. Drescher, H. Zhang, G. Coussanes, Y. Chen, N. Maulide

Glutathione-Inspired Octapeptides as Chelating Agents for Lead [MC-128]

Luca Sauser, University of Zurich

M. Shoshan*

Discovery of new inhibitors of human divalent metal transporter hDMT and hZIP8 by fragment-based lead discovery from GDB17 database [MC-129]

Céline Schuppisser, University of Bern

J. Pujol-Giménez, M. Poirier, S. Bühlmann, R. Bhardwaj, M. Awale, R. Visini, S. Javor, J. L. Reymond*, M. A. Hediger*

Modelling the active site of New Delhi Metallo- β -lactamase-1 [MC-130]

Justine Schwarte, University of Fribourg

K. M. Fromm*

Development of Positron-Emission Tomography and Fluorescent Tracers for the Imaging of Calcium Sensing Receptors (CaSR) in Parathyroid Glands [MC-131]

Daria Sokolova, University of Basel

M. Lochner*

Development of a single-molecule approach to observe ubiquitination dynamics in defined chromatin states [MC-132]

Alexandra Teslenko, EPFL Lausanne

B. Fierz*

Designing of new anticancer peptides using a Genetic Algorithm and Machine Learning [MC-133]

Elena Zakharova, University of Bern

D. Erzina, J. L. Reymond*

Synthesis of new building blocks from the chemical universe database GDB [MC-134]

Aline Carrel, University of Bern

J. L. Reymond*

**Organic Chemistry [OC]
Virtual Poster Session****Selective C-H azidation of amino acids and peptides [OC-101]**

Emmanuelle Allouche, EPFL Lausanne

R. Simonet-Davin, J. Waser*

Desymmetrization of Difluoromethylene Groups by C-F Bond Activation [OC-102]

Willi Amberg, ETH Zurich

J. F. Hartwig*

Imaging Membrane Tension During Endocytosis [OC-103]

Lea Assies, University of Geneva

F. Piazzolla, V. Mercier, J. López-Andarias, A. Roux, N. Sakai, S. Matile*

Exploring Bimetallic Cooperation for the Rational Design of Nucleophilic Silyl Reagents [OC-104]

Sophia Belrhomari, University of Bern

L. J. Bole, E. Hevia*

Sigma- or pi-dimer? [OC-105]

Annika Bernhardt, University of Zurich

C. M. Cruz, O. Blacque, M. Juríček*

Alkynyl hypervalent iodine reagents: improved synthesis for their in situ generation [OC-106]

Julien Borrel, EPFL Lausanne

J. Waser*

Organophotocatalytic Aerobic Oxygenation of Phenols in a Visible-Light Continuous-Flow Photoreactor [OC-107]

Thomas Buchholz, University of Basel
D. Miladinov, J. Wellauer, J. Schütz, R. Stemmler, J. A. Medlock, W. Bonrath, C. Sparr*

Cyclopentadienone Iron Complex Catalyzed Hydrogenation of Ketones: An Operando Spectroscopic Study Using Pressurized Sample Infusion Electrospray Ionization Mass Spectrometry [OC-108]

André Bütikofer, ETH Zurich
V. Gorbachev, P. Chen*

IBM RoboRXN: Automating Chemical Synthesis Remotely with AI and Cloud [OC-109]

Alessandro Castrogiovanni, IBM Research Europe
M. Manica, A. C. Vaucher, A. Cardinale, A. Sobczyk, T. Laino

Nonacethrene Unchained: A Method Toward Contorted Nanocarbons [OC-110]

Daniel Čavlovič, University of Zurich
P. Ravat, D. Häussinger, O. Blacque, M. Juríček *

Synthesis of Highly Functionalized Cyclopentanes through Atom Transfer Radical Addition Cyclization Cascade [OC-111]

Dace Cirule, University of Bern
P. Renaud*

Nickel-Catalyzed Asymmetric Synthesis of α -Arylamides [OC-112]

Sergio Cuesta-Galisteo, University of Zurich
J. Schörghener, X. Wei, E. Merino, C. Nevado*

Synthesis of chiral benzylic amino alcohol: Molecular tether approach [OC-113]

Ashis Das, EPFL Lausanne

Development and Molecular Understanding of Cyanation of Aryl Boronic Acids Through High-Throughput Experimentation and Data Analysis [OC-114]

Jordan De Jesus Silva, ETH Zurich
N. Bartalucci, B. Jelier, S. Grosslight, T. Gensch, C. Schünemann, B. Müller, P. Kamer, M. S. Sigman, C. Copéret*, A. Togni*

Stereoselective Synthesis of Hetero-Vinylbenziodoxolones Reagents and Their Reactivity as Oxy-Allyl Cation Synthetic Equivalents [OC-115]

Nina Declas, EPFL Lausanne
J. Waser*

Atom economic difunctionalisation: the addition of acid chlorides across unsaturated C–C bonds [OC-116]

Elliott Denton, ETH Zurich
Y. H. Lee, S. Roediger, P. Böhm, M. Fellert, B. Morandi*

At the Core of Dynamic Polymers: The Self-Assembly of Twisted Aryl Amines [OC-117]

Melissa El Bitar Nehme, University of Zurich
M. Rickhaus*

Through Bond and Space: Curved Light Harvesting Arrays [OC-118]

Lucia Gallego, University of Zurich
M. Rickhaus*

Ir(III)-catalyzed C(sp³)-H directed amidation for the synthesis of 1,2-aminoalcohols [OC-119]

Andrea Geraci, University of Basel
K. Antien, M. Parmentier, O. Baudoin*

Transmetalation of Monocyclometalated Gold(III) Complexes with Boronic Acids: Novel Selectivity and Mechanistic Insight [OC-120]

Jorge González, University of Zurich
F. Verdugo, J. L. Mascareñas, F. López, C. Nevado*

Flipper and flap: two mechanosensitive probes [OC-121]

Maxime Vonesch, University of Geneva
J. Garcia-Calvo, J. López-Andarias, N. Sakai, S. Saito*, S. Matile*

Introduction of Peripheral Side Groups to the Octulene Scaffold [OC-122]

Thomas Kader, University of Zurich
M. Rickhaus*

The Taming of Helical Triplet Diradical [OC-123]

Moheb Karbasiyoun, University of Zurich
Catalyst-free Photochemical C(sp³)-H Arylation of Amides in a Solvent-Caged EDA Complex [OC-124]
Jaspreet Kaur, Universität Regensburg
A. Shahin, M. Swierczewski*

Selective Tetrafunctionalizations on Phenolic Macrocycles: Diversifying the Calix[4]arene Family [OC-125]

Suren Nemat, University of Basel
K. Tiefenbacher*

Organic Building Blocks for 2D Interwoven Molecular Textiles [OC-126]

Camiel Kroonen, University of Basel
M. Mayor*

Accessing Monosubstituted Cyclopentadienyl Rhodium(I) and Iridium(I) Complexes by a Simultaneous Nucleophilic Addition-Metalation Approach to Fulvenes [OC-127]

Aragorn Laverny, EPFL Lausanne
N. Cramer*

Structure and Reactivity of New Cyclic Alkynyl Hypervalent Iodine Reagents [OC-128]

Elliott Le Du, EPFL Lausanne
T. Duhaill, M. D. Wodrich, R. Scopelliti, F. Fadaei-Tirani, E. Anselmi, E. Magnier*, J. Waser*

Inhibitors of Thiol-Mediated Uptake [OC-129]

Bumhee Lim, University of Geneva
Y. Cheng, A. Pham, T. Kato, D. Moreau, J. López-Andarias, L. Zong, N. Sakai, S. Matile*

Oligomers of Cyclic Oligochalcogenides for Enhanced Cellular Uptake [OC-130]

Rémi Martinet, University of Geneva
J. López-Andarias, S. Tawfik, Q. Laurent, N. Sakai, S. Matile*

N-heterocyclic substituted aldehydes in organocatalyzed conjugate addition reactions [OC-131]

Jasper Möhler, ETH Zurich
H. Wennemers*

A novel functionalization of pH-sensitive diaza[4]helicenes based on metal carbene insertion mechanism [OC-132]

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

Asymmetric Catalysis by Chiral Cp^xCo^{III} Complexes [OC-133]

Kristers Ozols, EPFL Lausanne
N. Cramer*

 α -Diazo-yonesters - a Versatile Scaffold Towards Formation of Hydroxypyrroles & Hydroxypyrazoles [OC-134]

Romain Pertschi, University of Geneva
A. de Aguirre, C. Besnard, A. I. Poblador Bahamonde, J. Lacour*

Peptide Stapling with Anion- π Catalysts [OC-135]

Anh-Tuan Pham, University of Geneva
N. Sakai, S. Matile*

Organic Molecules with Inverted Gaps between First Excited Singlet and Triplet States and Appreciable Fluorescence Rates [OC-136]

Robert Pollice, University of Toronto
P. Friederich, C. Lavigne, G. dos Passos Gomes, A. Aspuru-Guzik*

Simple carbonyl α -deuterations via keteneiminium intermediates [OC-137]

Vincent Porte, University of Vienna
H. Zhang, G. Di Mauro, M. Schupp, D. Kaiser, N. Maulide*

Asymmetric epoxidation and cyclopropanation using a catalytically formed chiral auxiliary [OC-138]

Mikus Purins, EPFL Lausanne
J. Waser*

Cu(I)-Catalyzed gem-Amino Alkynylation of Diazo Compounds: Straightforward Synthesis of Fluorinated Propargylic Amines [OC-140]

Nieves Ramirez, EPFL Lausanne
G. Pisella, J. Waser*

Diversification of Phosphine Ligands by Formal Substitution at Phosphorus [OC-141]

Sven Roediger, ETH Zurich
B. Morandi*

Reversible Michael Acceptors for Thiol Mediated Cellular Uptake and Inhibition [OC-142]

Inga Shybeka, University of Geneva
B. Lim, A. Pham, N. Sakai, S. Matile*

Induced Axial Chirality by a 2,5-Substituted Cofacial *para*-Phenylene-Ethynylene Framework [OC-143]

Eric Sidler, University of Basel
J. Malinčik, M. Mayor*

Radical azidation of cyclopropenes for the synthesis of quinolines [OC-144]

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

Optimized iminium-catalyzed 1,4-reductions inside the resorcinarene capsule: Achieving >90% ee with proline as catalyst [OC-145]

Daria Sokolova, University of Basel
K. Tiefenbacher*

Non-innocent electrophiles unlock exogenous base-free coupling reactions [OC-146]

Georgios Toupalas, ETH Zurich
B. Morandi*

Enabling Cyclization Strategies through Carbonyl Ylide Mediated Synthesis of Malonate Enol Ethers [OC-147]

Júlia Viñas-Lóbez, University of Geneva
G. Levitre, A. de Aguirre, C. Besnard, A. I. Poblador-Bahamonde,
J. Lacour*

Methylthio-benzothiazole based self-assembled monolayer for quantitative functionalisation by thiolated substrates. [OC-148]

David Vogel, University of Basel
D. Scherrer, G. Prone, M. Mayor*, E. Lörtscher*

Oxidative Ring-Opening Reactions of Aminocyclopropanes [OC-149]

Ming-Ming Wang, EPFL Lausanne
J. Waser*

Synthesis of Carpyridines [OC-150]

Joseph Woods, University of Zurich
M. Rickhaus*

Atropo-Enantioselective Oxidation-Enabled Iridium(III)-Catalyzed C–H Arylations with Aryl Boronic Esters [OC-151]

Łukasz Woźniak, EPFL Lausanne
N. Cramer*

Direct Photochemical C(sp³)-H Fluorination of Complex Molecules via a Photosensitized Auxiliary Approach [OC-152]

Shahboz Yakubov, Universität Regensburg
X. Tian, M. Swierczewski*

Synthesis of Twisted Triaryl Amines [OC-153]

Kai Zhang, ETH Zurich
M. El Bitar Nehme, M. Rickhaus*

Photo-induced Charge Transfer in Azapyrene-Tetrathiafulvalene Triads [OC-154]

Ping Zhou, University of Bern
U. Aschauer, T. Feuerer, R. Häner, S. Liu*

Palladium(0)-Catalyzed Enantioselective Intramolecular Arylation of Enantiotopic Secondary C–H Bonds [OC-155]

Marco Zuccarello, University of Basel
R. Melot, D. Cavalli, N. Niggli, M. Devereux, T. Bürgi, O. Baudoin*

**Physical Chemistry [PC]
Virtual Poster Session****Mapping Techniques in Nonadiabatic Quantum Dynamics [PC-102]**

Graziano Amati, ETH Zurich
J. O. Richardson*

Cold ion chemistry within a Rydberg-electron orbit: Test of the spectator role of the Rydberg electron in the He(*n*) + CO → C(*n'*) + O + He reaction [PC-103]

Fernanda B.V. Martins, ETH Zurich
V. Zhelyazkova, C. Seiler, F. Merkt*

Size- and time-resolved electron solvation following below band gap photoexcitation of neutral water clusters [PC-104]

Loren Ban, ETH Zurich

C. W. West, E. Chasovskikh, T. E. Gartmann, B. L. Yoder, R. Signorell*

Super-resolution microscopy with cucurbituril-encapsulated fluorophores [PC-105]

Liza Briant, University of Geneva

A. Fürstenberg*

Excited-state dynamics of organic molecules at liquid-phospholipid-liquid interfaces [PC-106]

Darya Budkina, University of Geneva

J. Sissaoui, E. Vauthey*

Ionization energy of the metastable 2^1S_0 state of ^4He from Rydberg-series extrapolation [PC-107]

Gloria Clausen, ETH Zurich

P. Jansen, S. Scheidegger, J. A. Agner, H. Schmutz, F. Merkt*

Femtosecond broadband fluorescence upconversion spectroscopy to study the planarization dynamics of 9,10-bis(phenylethynyl)anthracene [PC-108]

Ina Fureraj, University of Geneva

E. Vauthey*

Electric Field Gradient calculation within Frozen-Density Embedding Theory [PC-109]

Yann Gimbal-Zofka, University of Geneva

T. A. Wesolowski*

Core-valence attosecond transient absorption spectroscopy of polyatomic molecules [PC-110]

Nikolay Golubev, EPFL Lausanne

J. Vaníček, A. I. Kuleff

Investigation of Hydrogen Transfer Catalytic Cycle of (Cyclopentadienone)iron Complexes by Cryogenic Ion Vibrational Predissociation (CIVP) Spectroscopy [PC-111]

Vladimir Gorbachev, ETH Zurich

A. Bütikofer, P. Chen*

Low-energy reactive collisions of all stable molecular hydrogen isotopologues: branching ratios, deviation from Langevin behavior and kinetic energy analysis of the products. [PC-112]

Raphaël Hahn, ETH Zurich

K. Höveler, J. Deiglmayr, J. A. Agner, F. Merkt*

High-Resolution Spectroscopy in Argon using a Long-Pulse Fourier-Transform Limited Laser System [PC-113]

Holger Herburger, ETH Zurich

U. Hollenstein, F. Merkt*

Polymer GUVs for Studying Compartmentalized Biological Systems [PC-114]

Lukas Heuberger, University of Basel

E. dos Santos, R. Wehr, D. Hürlimann, W. Meier*, C. Palivan*

High-Resolution Spectroscopy in Supersonic Beams using a QCL Dual-Comb Spectrometer [PC-115]

Urs Hollenstein, ETH Zurich

J. A. Agner, P. Allmendinger, A. Hugi, K. Keppler, M. Mangold, F. Merkt*, M. Quack*

Ionization Energies of Para- H_2 from Zero-Quantum-Defects Positions [PC-116]

Nicolas Hölsch, ETH Zurich

I. Doran, F. Merkt*

In-operando morphological changes of P3HT studied by vibrational spectroscopy in organic electrochemical transistors [PC-117]

Isabelle Holzer, University of Bern

P. Cavassin, N. Banerji*

High Resolution Infrared Spectroscopy of Aziridine-2-Carbonitrile ($\text{C}_3\text{H}_4\text{N}_2$) [PC-118]

Karen Keppler, ETH Zurich

S. Albert, C. Manca Tanner, J. Stohner, M. Quack*

Spectroscopic Studies of Ion-Pair States of Polyatomic Molecules [PC-119]

Carla Kreis, ETH Zurich

U. Hollenstein, F. Merkt*

Mechanism of Material Transfer from Ion Sensing Component-Loaded Nanoemulsions: An Electrochemical Quartz Crystal Microbalance and Thin Film Coulometry Study [PC-121]

Canwei Mao, University of Geneva

Y. Soda, K. J. Robinson, T. Forrest, E. Bakker*

Implementation of a novel transporter system into artificial membranes [PC-122]

Moritz Muthwill, University of Basel

A. Krywko-Cendrowska, S. Yorulmaz Avsar, R. Wehr,

D. Sokolova, K. Tiefenbacher*, C. Palivan*

On the absolute photoionization cross section of the fulvenone ketene [PC-123]

Zeyou Pan, Paul Scherrer Institute, Villigen

A. Bodi, J. A. van Bokhoven*, P. Hemberger*

Ultrafast Charge Dynamics in p-Doped Conjugated Polymers – Glycol functionalized Polythiophene P(g4 2T-T) versus workhorse P3HT [PC-124]

Eva Röck, University of Bern

D. Tsokkou, C. Müller, E. Järsvall, N. Banerji*

Measurements of np - $2s$ transitions in the hydrogen atom [PC-125]

Simon Scheidegger, ETH Zurich

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

Precision infrared spectroscopy using a fibre link for the distribution of the Swiss primary frequency standard [PC-126]

Aleksandr Shlykov, University of Basel

M. F. Roguski, M. Sinhal, Z. Meir, M. Bertrand, J. Faist, F. Merkt,

E. Heiri, D. Husmann, J. Morel*, S. Willitsch*

Probing Liquid Interfaces with Room-Temperature Ionic Liquids Using the Excited-State Dynamics of a Cationic Dye [PC-127]

Jihad Sissaoui, University of Geneva

D. S. Budkina, E. Vauthey*

Introducing Order and Disorder into Inverse Opals [PC-128]

Jansie Smart, University of Fribourg

M. Lattuada*

Bridging Au₂₅(SR)₁₈ nanoclusters with a new chiral dithiol to form extremely stable dimers and trimers. [PC-129]

Michal Swierczewski, University of Geneva
F. Cousin, E. Banach, A. Ziarati, R. Azoulay, T. Bürgi*, L. Lee*

Bimolecular Photoinduced Electron Transfer in Non-Polar Solvents [PC-130]

Pragya Verma, University of Geneva
E. Vauthey*

Thermal Decomposition Mechanism of Vanillin, a Lignin Model Compound [PC-131]

Xiangkun Wu, Paul Scherrer Institute, Villigen
S. Bjelič, P. Hemberger, A. Bodi*

Conformationally controlled ionic Diels-Alder reactions in the gas phase [PC-132]

Lei Xu, EPFL Lausanne
A. Kilaj, P. Stranak, J. Wang, J. Küpper*, S. Willitsch*

New methods for studying state and conformational effects in chemi-ionisation reactions in the gas phase [PC-133]

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

**Polymers, Colloids & Interfaces [PI]
Virtual Poster Session****Conjugated Microporous Polymers Using a Copper-Catalyzed [4+2] Cyclobenzannulation Reaction: Promising Materials for Iodine and Dye Adsorption [PI-101]**

Noorullah Baig, Gulf University for Science and Technology
S. Shetty, B. Alameddine*

PLA-lignin films for sustainable food packaging [PI-102]

Alice Boarino, EPFL Lausanne
H. Klok*

Understanding the role of monomer-monomer interactions in the formation of semi-crystalline surface patterns from trimeric DNA macromolecules [PI-103]

Vincenzo Caroprese, EPFL Lausanne
C. Tekin, V. Cencen, G. Fantner*, M. M. C. Bastings*

pH Responsive Microgels as Reversible “on demand” Cation Carriers [PI-104]

Vittoria Chimisso, University of Basel

Mechano-pigments for high dynamic range mechano-sensing in polymeric materials [PI-105]

Jessica Clough, Adolphe Merkle Institute, Fribourg
S. Schrettl, C. Weder*

Solvent-free synthesis of stretchable electrodes for application in green stacked dielectric elastomer actuators [PI-106]

Patrick Danner, Empa
M. Iacob, I. Burda, B. Rieger, F. Nüesch, D. M. Opris*

One-pot Synthesis of Amphiphilic ABC Triblock Copolymer PEO-*b*-PEHO_x-*b*-PEtOz and its Self-Assembly into Nanoscopic Asymmetric Polymersomes [PI-107]

Davy Daubian, University of Basel
A. Fillion, J. Gaitzsch, W. Meier*

Synthesis of polymeric particles with multiple lobes [PI-108]

Kata Dorbic, University of Fribourg
M. Lattuada*

Supramolecular Assembly of Sugar Modified Disubstituted Pyrene Oligomer [PI-109]

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

Covalent Triazine Frameworks Incorporating Charged Polypyrrole Channels for High-Performance Lithium-Sulfur Batteries [PI-110]

Ahmed Elabd, University of Fribourg
J. Kim, A. Coskun*, J. Wook Choi*

Controlled Enzyme (Co)Immobilization by Simple and Stable Adsorption of Polymer-Enzyme Conjugates within Porous Silica [PI-112]

Nicolas Ghéczy, ETH Zurich
P. Walde*

Easy synthesis of nano- and micro-sized light-responsive cargo carrier for organ-on-a-chip device [PI-113]

Sètuhn Jimaja, Adolphe Merkle Institute, Fribourg
N. Bruns*

Cyclodextrine as a tool to follow the blue-to-red transition of polydiacetylenes [PI-114]

Levente Juhasz, University of Geneva
A. Fürstenberg*

Plasticization of a rigid metallosupramolecular polymer network [PI-115]

Franziska Marx, Empa
S. Schrettl*, C. Weder*

Highly porous nanofiber sponge immobilized MOF for efficient CO₂ capture [PI-116]

Gioele Mol, Zurich University of Applied Sciences ZHAW
C. Adlhart*

Exploiting phase transitions in polymer bilayer actuators [PI-117]

Livius Muff, Adolphe Merkle Institute, Fribourg
A. Mills, K. Daltorio, C. Weder*

Synthesis of Covalent Chitosan-Based Derivatives for Gene Delivery [PI-118]

Laura Nicolle, EPFL Lausanne
C. M. Journot, P. Robin, J. Casper, P. Detampel, M. Williman, H. Grisch-Chan, B. Thöny, S. Gerber-Lemaire*, J. Huwyler*

Functionalization of Self-Assembled Fibers via Copper-Free “Click” Chemistry [PI-119]

Erich Peters, University of Bern
S. M. Langenegger, R. Häner*

Electrospun chitosan nanofiber sponge for filtration of microplastics [PI-120]

Patricia Risch, Zurich University of Applied Sciences ZHAW
C. Adlhart*

Multifunctional silica-based sensors for real-time viral screening [PI-121]

Perrine Robin, EPFL Lausanne
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Stabilization of nanoparticle emulsion based ion selective optodes through zwitterionic surfactants [PI-122]

Kye Robinson, University of Geneva
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In situ polymerization in a microfluidic chip [PI-123]

Marco Rocca, IBM Research Europe
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A. Anastasaki*

AIE-Active DNA Conjugates Self-Assemble into DNA-Addressable Vesicles [PI-125]

Simon Rothenbühler, University of Bern
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Suchetha Shetty, Gulf University for Science and Technology
N. Baig, B. Alameddine*

Molten Salt Templated Synthesis of Covalent Isocyanurate Frameworks with Tunable Morphology and High CO₂ Uptake Capacity [PI-127]

Kyung Seob Song, University of Fribourg
S. N. Talapaneni, T. Ashirov, A. Coskun*

Supramolecular Assembly of Pyrene-DNA Conjugates into Vesicles [PI-128]

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

Shining light on surface-initiated organocatalyzed atom transfer radical polymerization [PI-129]

Sophia Thiele, EPFL Lausanne
H. Klok*

The Role of Hydrodynamic Interactions on the Aggregation Kinetics of Sedimenting Colloidal Particles [PI-130]

Lorenzo Turetta, University of Fribourg
M. Lattuada*

Tailoring polymer dispersity by (PET)-RAFT polymerization: a versatile approach [PI-131]

Júlia Viñas-Lóbez, University of Geneva
R. Whitfield, A. Anastasaki*

Self-healable dielectric elastomer actuators operated at low electric fields [PI-132]

Johannes von Szczepanski, Empa
M. Bajc, D. M. Opris*

Chiral nano- and microscopic vesicles composed of fully amorphous isotactic block copolymers [PI-133]

Riccardo Wehr, University of Basel
E. dos Santos, M. Muthwill, V. Chimisso, J. Gaitzsch, W. Meier*

Drug loaded hollow mesoporous silica nanoparticles–DNA self-assembly for responsive antimicrobial coatings [PI-134]

Philippe Yep, University of Fribourg
E. Jean-Pierre, K. M. Fromm*

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