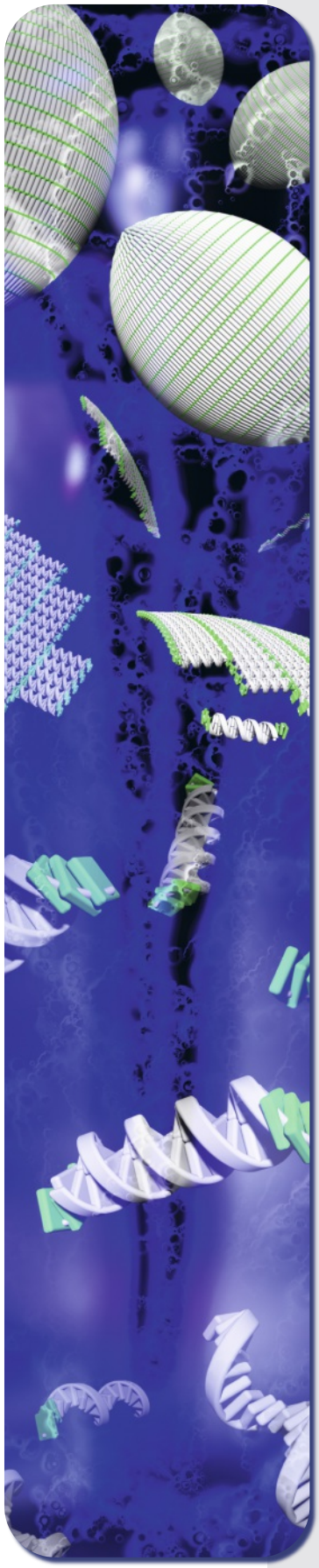


UNIVERSITÄT BERN

SCS
Swiss Chemical Society

Online Conference
Tuesday, 25. August 2020, 08:30-18.30

SCS Fall Meeting 2020

- 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)

scg.ch/fallmeeting/2020

Pictures left: Illustration of vesicle formation via supramolecular assembly of amphiphilic DNA. Graphics by Simon Rothenbühler, Simon M. Langenegger, and Robert Häner, Department of Chemistry and Biochemistry, University of Bern
Pictures bottom: Illustration of the virtual Fall Meeting 2020 conference location by SCS

doi:10.2533/chimia.2020.585 Chimia 74 (2020) 585–608

Welcome to the 2020 Fall Meeting of the Swiss Chemical Society (SCS)

Dr. Hans Peter Lüthi

Prof. Silvio Decurtins

Prof. Stefan Willitsch

On behalf of the Organizing Committee and the Division of Fundamental Research of the Swiss Chemical Society, we welcome you to the 2020 Fall Meeting, held as a virtual meeting & virtual exhibition. The decision taken early on not to cancel the event, but to setup an Online Conference, has since paid off: We received more than 400 abstracts for short talks or virtual posters, could welcome more than ten exhibitors, and found sponsors for all of the nine thematic sessions covering all of the chemistry! This is well beyond what we could expect, and it shows that the Fall Meeting is a welcome opportunity for our young scientists to communicate their results.

Once registered (online on: *scg.ch/fallmeeting/2020*), you are invited to enter the four virtual rooms. In the 'Plenary Session room', you can follow the Award Lectures (Werner and Sandmeyer Prizes, the Industrial Science Awards, and the Paracelsus Price). The 'Parallel Sessions room' offers the platforms for the nine thematic sessions, most with two Invited Lectures and ten Short Talks presented by students. For the first time, there is a session on Chemistry and the Environment. It addresses research on issues such atmospheric, aquatic and soil chemistry, and the effect of this chemistry on living organisms. We wish the newcomer every success!

The 'Poster Session Rooms' host the nine virtual Poster Sessions, accessible during the entire week. Rather than to display traditional posters, the participants prepared a few slides on their research and present these in a short video. As in the 'Exhibition Room', where you can visit the booths of our exhibitors, there are means of interacting with the presenters online.

The meeting ends with the announcement of the winners of the 'New 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 which went along with us for many years. We thank all the members of the Organizing Committee for their great support and especially the staff of the Swiss Chemical Society, who laid the cornerstone for a successful online meeting. We invite you to browse through the program and look forward to meet you in the virtual rooms and online platforms of the 2020 Fall Meeting.

Dr. Hans Peter Lüthi
Vice Chairman of the
Organizing Committee

Prof. Silvio Decurtins
Chairman of the
Organizing Committee

Prof. Stefan Willitsch
Chairman of the Division
of Fundamental Research
and Co-Chairman of
the Organizing Committee

PROGRAM OVERVIEW, TUESDAY, 25TH AUGUST 2020

Interactive program incl. abstracts of all lectures, talks and virtual posters on *http://scg.ch/fallmeeting/2020*

Time	Program Item
08.00	Open virtual conference room
08.30	Welcome and conference opening ***Prof. Silvio Decurtins***, University of Bern and ***Dr. Hans Peter Lüthi***, SCS Foundation Co-Chairs of the SCS Fall Meeting 2020
Morning Plenary Session (Award Lectures)	
08.45	Werner Prize Lecture 2020 ***Prof. Konrad Tiefenbacher***, University of Basel/ETH Zurich «Molecular capsule catalysis: Ready to address current challenges in synthetic organic chemistry?»
09.15	Sandmeyer Award Lecture 2020 ***Dr. Andreas Schuster*** as representative of the Ipatasertib Team at F. Hoffmann La-Roche and ***Dr. Christoph Strasser***, Dottikon Exclusive Synthesis AG «Development of the Commercial Manufacturing Process for Ipatasertib»
09.45	Short Break
Morning Parallel Sessions	
10.00	**Invited/Sponsored Lecture** (30min) and **Short Talks** (15min) Topics: Analytical Sciences, Catalysis Science & Engineering, Computational Chemistry, Chemistry and the Environment, Inorganic & Coordination Chemistry, Medicinal Chemistry & Chemical Biology, Organic Chemistry, Physical Chemistry and Polymers, Colloids & Interfaces
Lunch Break and Poster Session	
11.45	**Virtual Poster Sessions** Read abstracts, watch short videos and interact with the presenters *via* mail, social media or skype. The poster session is open from Mon, 24.08.2020 12.00h to Fri, 28.08.2020 18.00h. **Virtual Commercial Exhibition** Visit the virtual boots and inform yourself about the latest developments of our partners Participate in the online quiz and get the chance to win 2x 100 CHF in cash.
12.30	youngSCS General Assembly
Afternoon Parallel Sessions	
13.30	**Invited/Sponsored Lecture** (30min) and **Short Talks** (15min) Topics: Analytical Sciences, Catalysis Science & Engineering, Computational Chemistry, Chemistry and the Environment, Inorganic & Coordination Chemistry, Medicinal Chemistry & Chemical Biology, Organic Chemistry, Physical Chemistry and Polymers, Colloids & Interfaces
Afternoon Plenary Session (Award Lectures)	
15.30	SCS Industrial Science Award Lecture 2020 ***Dr. Denis Jacoby***, Firmenich SA «Tailored Catalysis for the F&F Industry»
16.00	SCS Senior Industrial Science Award Lecture I/2020 ***Dr. Frank Petersen***, Novartis Pharma AG «Natural Product Sciences in Modern Drug Discovery and Paths to the Future»
16.30	Short Break
16.45	SCS Senior Industrial Science Award Lecture II/2020 ***Dr. Hasane Ratni***, F. Hoffmann-La Roche Ltd. «Discovery of a new medicine Risdiplam, a Survival of Motor Neuron-2 (SMN2) gene splicing modifier for the treatment of Spinal Muscular Atrophy (SMA)»
16.45	Paracelsus Prize Lecture 2020 ***Scott E. Denmark***, University of Illinois, Urbana (USA) «Discovery and Optimization of Enantioselective Catalysts through Chemoinformatics»
SCS Announcements and Ceremony Session	
17.45	**SCS Announcements** **Helvetica Prize of the Swiss Chemical Society 2020** (best published papers of PhD/Postdocs 2019/20)
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. Thomas Netscher, Principal Scientist at DSM Nutritional Products
18.30	End of the conference

General Information

Date: August 25, 2020, 08.30–18.30 h
Location: Online Meeting
Host: University of Bern
Department of Chemistry and Biochemistry
Freiestrasse 3
3012 Bern
Website: *http://scg.ch/fallmeeting/2020*

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

Organizing Committee

Chairmen
Prof. Silvio Decurtins
Department of Chemistry and Biochemistry, University of Bern
silvio.decurtins@dcb.unibe.ch

Dr. Hans Peter Lüthi
ETH Zurich and SCS Foundation
luethi@scg.ch

Session Chairs
Analytical Sciences
– Prof. Stefan Schürch, University of Bern
– 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 Zurich
– Prof. Jeremy Richardson, ETH Zurich
Inorganic & Coordination Chemistry
– Prof. Marinella Mazzanti, EPF Lausanne
– Prof. Kay Severin, EPF Lausanne
– Prof. Roger Alberto, University of Zurich
Organic Chemistry
– Prof. Pablo Rivera-Fuentes, EPF Lausanne
– Prof. Jason Holland, University of Zurich
– Prof. Michal Juríček, University of Zurich
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. Walter Caseri, ETH Zurich
– Dr. Dominik Brühwiler, ZHAW Wädenswil
Chemistry and the Environment
– Prof. Kathrin Fenner, Eawag Dübendorf und University of Zurich
– Prof. Tamar Kohn, EPFL Lausanne

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 9 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.

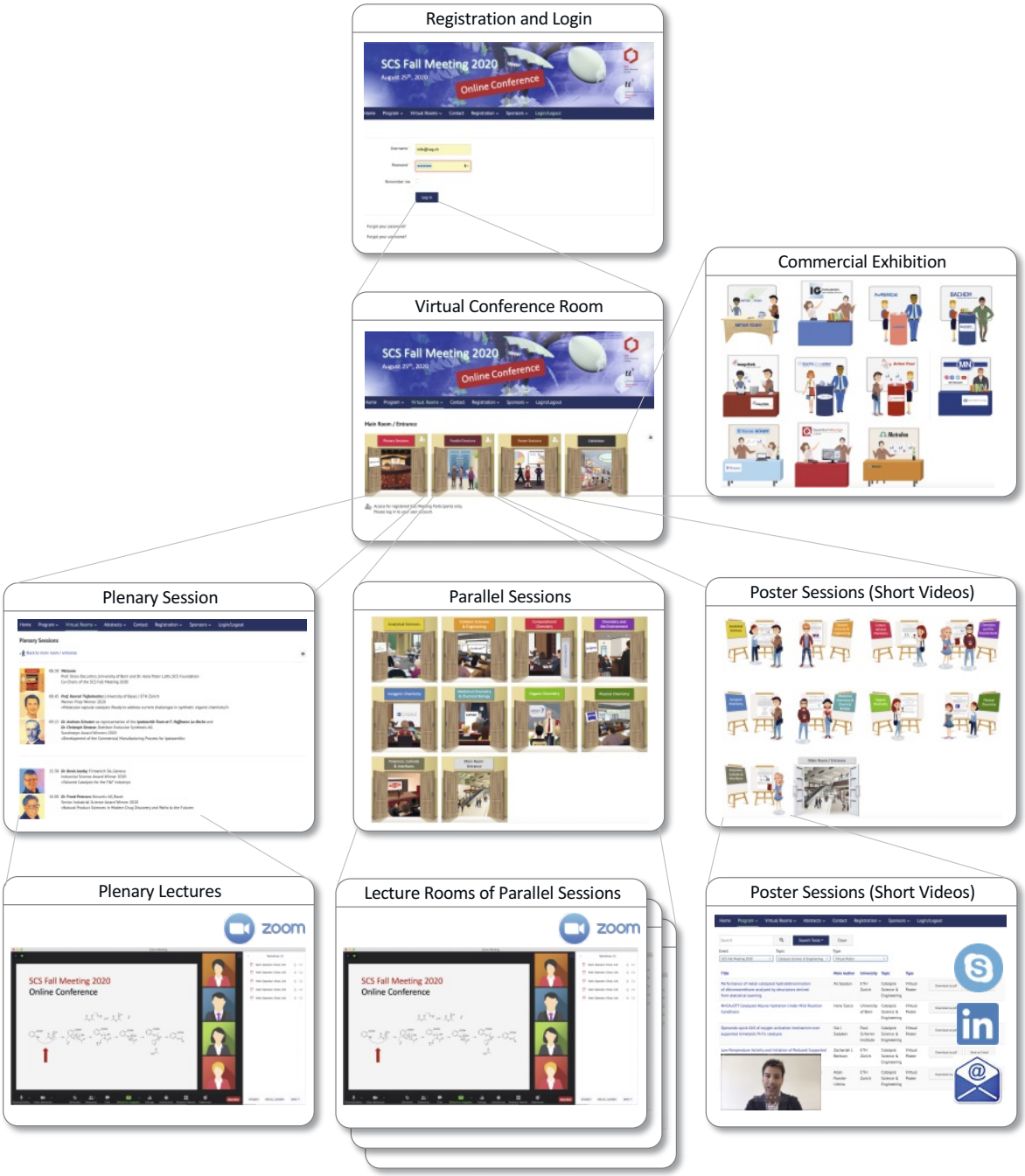
Access the Virtual Conference
Select the menu item 'Virtual Rooms' on the conference website to open the entry point for the lecture sessions, the poster sessions and the exhibition.
The exhibition is accessible without a login. A participant profile is required to attend the scientific sessions.

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 consult the website:
zoom.us/download#client_4meeting

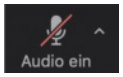
Virtual Poster Sessions / Short Videos
Poster presenters will introduce their research projects in short videos of max. 3 minutes. With this approach it will be easier for the audience to follow numerous presentations and to understand the key message of each project. Tools to interact with the presenter allow visitors to ask questions or to comment on the presented content. We offer email, skype or social media channels to interact with each other.

Interactive Program and Abstract Search
The website allows you to plan your conference day easily and interactively. 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.

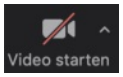
VIRTUAL CONFERENCE LOCATION



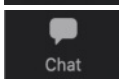
Rules for the online Lectures



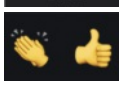
Audio on only for the speaker.
This function is managed by the operator



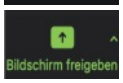
Deactivate the video function to reduce data transition.



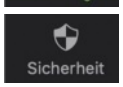
Send your question *via* chat to the speaker or
send a note to the operator that you would like to ask a question in the Q&A session at the end of each presentation



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 grants or free publication opportunities in the Junior Laureates issue of CHIMIA 4/2021.

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.

Covers of the 2018–2020 Junior Laureates Issues

Best Oral Presentation Award

The award is sponsored by Metrohm

The prizes are awarded 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: 18.00h in the plenary lecture room.

Prize for the winner of each of the nine, parallel sessions
– Cash contribution of CHF 500
– Travel voucher of CHF 1000 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

Winners of the Fall Meeting Best Oral Presentation Award 2019 at University of Zurich

Best Poster Presentation Award

The award is sponsored by DSM.

The prizes are awarded 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: 18.15h in the plenary lecture room.

Prize for the winner of each of the seven, 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. Thomas Netscher, Principal Scientist at DSM Nutritional Products Ltd., Basel

Winners of the Fall Meeting Best Poser Presentation Award 2019 at University of Zurich

Photos: Hans Peter Lüthi, SCS

Helvetica Prize of the Swiss Chemical Society 2020

The prize is awarded for the best published papers of PhD/Postdocs 2019/20 in *Helvetica Chimia Acta*. The 2020 prizes go to:
– ***Jérémy Vuilleumier,*** EPFL Lausanne,
Group of Prof. Sandrine Gerber
«Photocontrolled Release of the Anticancer Drug Chlorambucil with Caged Harmonic Nanoparticles»
– ***Valentina Galli,*** University of Geneva
Group of Prof. Nicolas Winssinger
«Caprin-1 Promotes Cellular Uptake of Nucleic Acids with Backbone and Sequence Discrimination»

Dr. Richard Smith, Managing Editor of Helvetica, will present the certificates to the two winners on August 25, 2020, at 17.50h in the virtual plenary room. Both winners will present their research in an elevator talk of 3 min each.

Winners of the Helvetica Prize 2019: Jovana Milic (third from left) and Kevin Wieland (fourth from left).
The prizes were presented by Wiley-VHCA's Managing Editor, Dr. Richard Smith, and the two Editors in Chief, Prof. Jeff Bode and Prof Christoph Copéret, both from ETH Zurich

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.

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ENDOWMENTS OF PARALLEL SESSIONS

METTLER TOLEDO	CLARIANT	syngenta
Analytical Sciences	Catalysis Science & Engineering	Chemistry and the Environment
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Organic Chemistry	Physical Chemistry	Polymers, Colloids & Interfaces

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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 August 25, 17:45h.
The quiz is open from August 10, 2020, to August 25, 2020, 14.30h.

Plenary Sessions

Award Lectures

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

Werner Prize Lecture 2020
Molecular capsule catalysis: Ready to address current challenges in synthetic organic chemistry? [PS-001]
August 25, 2020, 08.45–09.15h

Prof. Konrad Tiefenbacher, University of Basel / ETH Zurich
Awarded for his innovative and original research in the field of supramolecular catalysis with focus on catalysis inside supramolecular containers, so called 'capsules'.

Sandmeyer Award Lecture 2020
Development of the Commercial Manufacturing Process for Ipatasertib [PS-002]
August 25, 2020, 09.15–09.45h

Dr. Andreas Schuster, Dr. Caroline Maierhofer, Dr. Stephan Bachmann, Dr. Hans Iding, Dr. Christian Lautz, Dr. Régis Mondière, Dr. Philipp Schmidt, Dr. Isabelle Thomé, from the Ipatasertib Team at F. Hoffmann La-Roche, and ***Dr. Christoph Strasser*** from Dottikon Exclusive Synthesis AG
The Team is awarded for the development of an economical, scalable and sustainable process to produce Ipatasertib, an Akt kinase inhibitor currently tested in Phase III clinical trials for the treatment of metastatic castration-resistant prostate cancer and triple negative metastatic breast cancer.

SCS Industrial Science Award Lecture 2020
Tailored Catalysis for the F&F Industry [PS-003]
August 25, 2020, 15.30–16.00h

Dr. Denis Jacoby, Firmenich SA, Geneva
The award is given to honor his outstanding achievements at Firmenich especially the development of major new processes for several key perfumery ingredients that are manufactured on multi MT scale today.

SCS Senior Industrial Science Award Lecture I/2020
Natural Product Sciences in Modern Drug Discovery and Paths to the Future [PS-004]
August 25, 2020, 16.00–16.30h

Dr. Frank Petersen, Novartis Pharmaceuticals AG, Basel,
Awarded in recognition of his outstanding contributions in the field of natural product research over three decades that includes the investigations for several products on the market or in clinical evaluation, the integration of natural product based scaffolds classes in chemical biology for the identification of novel targets, but also the partnerships in microbial sourcing and in accessing isolated plant metabolites in Africa, China, and Thailand.

SCS Senior Industrial Science Award Lecture II/2020
Discovery of a new medicine Risdiplam, a Survival of Motor Neuron-2 (SMN2) gene splicing modifier for the treatment of Spinal Muscular Atrophy (SMA) [PS-005]
August 25, 2020, 16.45–17.15h

Dr. Hasane Ratni, F. Hoffmann-La Roche, Basel,
Awarded in recognition of his outstanding contributions to medicinal chemistry and his track record of delivering successful clinical development candidates resulting in five molecules entering human clinical trials. This includes the seminal work on RNA interaction with small molecules leading to the discovery of risdiplam.

Paracelsus Prize Lecture 2020
Discovery and Optimization of Enantioselective Catalysts through Chemoinformatics [PS-006]
August 25, 2020, 17.15–17.45h

Prof. Scott E. Denmark, University of Illinois, Urbana-Champaign (USA)
Awarded for his role as internationally recognized leader in the development of novel concepts of catalysis, of very useful synthetic methods, and insightful mechanistic investigations in organic chemistry.

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: Prof. Stefan Schürch, University of Bern
Dr. Hanspeter Andres, METAS

10:00 **Generation and physicochemical characterisation of ambient-like model aerosols in the laboratory: application in the intercomparison of automated PM monitors with the reference gravimetric method [AS-011]**
Konstantina Vasilatou, Federal Institute of Metrology METAS

10:30 **Transition metal FRET in the gas phase: a 5–20 Å range structural probe for gaseous biomolecular backbone structure [AS-013]**
Prince Tiwari, ETH Zurich
R. Zenobi*

10:45 **Combined Mass Spectrometry-Based Studies of Cellular Protein Complexes under Native Conditions [AS-014]**
Mariia Naumenko, ETH Zurich
R. Zenobi*

11:00 **Multi element particle detection and information gain from particle clustering: A case study of waste water treatment plants across Switzerland [AS-015]**
Kamyar Mehrabi, ETH Zurich
R. Kägi, A. Gundlach-Graham, D. Günther*

11:15 **Characterization of an Extreme Ultraviolet Hollow Cathode Lamp by means of Plasma Emission Spectroscopy [AS-016]**
Di Qu, Empa, Dübendorf/University of Zurich
D. Bleiner*

11:30 **Forensic Float Glass Fragment analysis and matching by means of Single-Pulse Laser Ablation Inductively Coupled Plasma Time of Flight Mass Spectrometry [AS-017]**
Pascal Becker, ETH Zurich
D. Günther*

13:30 **Digital Transformation in Research Laboratories [AS-021]**
Christoph Jansen, Mettler-Toledo GmbH

14:00 **Arsenic speciation in mice gut after chronic exposure from rice [AS-023]**
Teresa Chávez-Capilla, University of Bern
M. Mukherjee, M. Coll-Crespi, A. Mestrot*, S. Hapfelmeier*

14:15 **Analyzing glycans cleaved from a biotherapeutic protein using ultrahigh-resolution ion mobility spectrometry together with cryogenic ion spectroscopy [AS-024]**
Natalia Yalovenko, EPFL Lausanne
V. Yatsyna, P. Bansal, T. R. Rizzo*

14:30 **Electron-impact, high-resolution mass spectrometry for non-targeted analysis of the atmosphere [AS-025]**
Myriam Guillevic, Empa, Dübendorf
M. K. Vollmer, A. Guillevic, M. Hill, P. Schlauri, S. Reimann, L. Emmenegger, M. Guillevic*

14:45 **Highly sensitive, spatially resolved ^{230}Th–^{232}Th–^{234}U–^{238}U analysis using LA-ICPMS [AS-026]**
Chung-Che Wu, ETH Zurich
C. Shen, D. Günther, B. Hattendorf*

15:00 **Quantitative and sensitive elemental analysis using a novel high mass resolution laser ablation ionization mass spectrometer [AS-027]**
Coenraad de Koning, University of Bern
A. Riedo, V. Grimaudo, M. Tulej, R. Lukmanov, N. F. Ligterink, P. Wurz*

Catalysis Sciences & Engineering [CE]

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

10:00 **Selectivity Control in CO_2 Electroreduction through Rational Catalyst and Electrolyte Design [CE-011]**
Beatriz Roldan Cuenya, Fritz-Haber-Institute of the Max Planck Society

10:30 **A mechanistic study of carbon dioxide hydrogenation to methanol by *operando* XAS, XRD and SSITKA-FTIR techniques [CE-013]**
Maxim Zabilskiy, Paul Scherrer Institute (PSI), Villigen
V. Sushkevich, D. Palagin, M. Newton, M. Zabilskiy*, J. A. van Bokhoven*

10:45 **Palladium-Gallium Alloyed Nanoparticles on Silica: Metal Synergy Yields Highly Active Catalyst for Selective CO_2-to-Methanol Hydrogenation [CE-014]**
Scott Docherty, ETH Zurich
C. Copéret*

11:00 **Unveiling the promotional effect of nickel in indium-catalyzed CO_2 hydrogenation to methanol [CE-015]**
Matthias S. Frei, ETH Zurich
C. Mondelli, R. García-Muelas, N. López, O. V. Safonova, D. Curulla-Ferré, J. A. Stewart, J. Pérez-Ramírez*

11:15 **Operando Spectroelectrochemical Observation of Surface States and Active Sites in Chalcopyrite Photocathodes for Solar Water Reduction [CE-016]**
Yongpeng Liu, EPFL Lausanne
K. Sivula*, N. Guijarro*

11:30 **Surface over-layer formation and dynamics in the strong metal-support interaction state on supported metal catalysts [CE-017]**
Arik Beck, ETH Zurich
X. Huang, L. Artiglia, M. Zabilskiy, P. Rzepka, D. Palagin, M. G. Willinger*, J. A. van Bokhoven*

13:30 **Revealing the structural secrets of random catalyst packings [CE-021]**
Jennie von Seckendorff, Clariant
O. Hinrichsen

14:00 **Time-resolved spectroscopy of vanadia-based SCR catalysts under transient conditions [CE-023]**
Rob Jeremiah G. Nuguid, Paul Scherrer Institute (PSI), Villigen
M. Nachtegaal, D. Ferri, O. Kröcher*

14:15 **Atom-by-atom active site synthesis by liquid-phase atomic layer deposition [CE-024]**
Benjamin Le Monnier, EPFL Lausanne
L. M. Savereide, M. Kiliç, R. Schnyder, M. D. Mensi, U. Roethlisberger, J. Luterbacher*

14:30 **Metal-organic frameworks as kinetic modulators for branched selectivity in hydroformylation [CE-025]**
Patrick Gäumann, Paul Scherrer Institute (PSI), Villigen/ETH Zurich
G. Bauer, D. Ongari, D. Tiana, T. Rohrbach, G. Pareras, M. Tarik, B. Smit, M. Ranocchiari*

14:45 **A Polymerised Water Reduction Catalyst for Photo- and Electrocatalysis [CE-026]**
Franziska Rahn, University of Zurich
B. Probst, R. Alberto*

15:00 **Development of a Microfluidics-based Assay for the Directed Evolution of Artificial Metalloenzymes using a Cell Surface-Display Strategy [CE-027]**
Jaicy Vallapurackal, University of Basel
A. Stucki, T. R. Ward*, P. S. Dittrich*

Computational and Theoretical Chemistry [CC]

Session Endowment: Schrödinger GmbH
Chairs: Prof. Jürg Hutter, University of Zurich
Prof. Jeremy Richardson, ETH Zurich

10:00 **Learning how to do chemical reactions from data [CC-011]**
Alain Vaucher, IBM Research Europe
A. Cardinale, J. Geluykens, V. H. Nair, O. Schilter, P. Schwaller, A. Logallo, F. Zipoli, T. Laino*

10:30 **Resonance Effects in the Raman Optical Activity Spectrum of $[Rh(en)_3]^{3+}$ [CC-013]**
Thomas Weymuth, ETH Zurich
M. Reiher*

10:45 **Zooming in on the O-O Bond Formation – Novel Insights from *ab initio* Molecular Dynamics with Enhanced Sampling Techniques [CC-014]**
Mauro Schilling, University of Zurich
R. A. Cunha, S. Luber*

11:00 **Using Ultrafast Spectroscopy and Computer Simulations to Re-examine Our Picture of Photoinduced Electron Transfer [CC-015]**
Christopher Rumble, University of Geneva
E. Vauthey*

11:15 **On-the-fly ab initio semiclassical evaluation of vibronic spectra at finite temperature [CC-016]**
Tomislav Begušić, EPFL Lausanne
J. Vaníček*

11:30 **Ionization of Water as an Effect of Quantum Delocalization at Aqueous Electrode Interfaces [CC-017]**
Jinggang Lan, University of Zurich
V. V. Rybkin, M. Iannuzzi

13:30 **Enabling Drug Discovery with an Integrated Computational Approach. A Case Study in Schrödinger's Molecular Design Platform [CC-021]**
Tim Knehans, Schrödinger GmbH

14:00 **Kinetic reweighting made easy – An integrator independent dynamic reweighting algorithm for biased simulations [CC-023]**
Stephanie M. Linker, ETH Zurich
R. G. Weiss, S. Riniker*

14:15 **Atomistic simulations of catalytic confined environments from supramolecular systems to biomass conversion [CC-024]**
Giovanni Maria Piccini, ETH Zurich/USI Lugano

14:30 **Simulating the Ghost: Quantum Dynamics of Solvated Electron [CC-025]**
Vladimir Rybkin, University of Zurich

14:45 **Designing Singlet Fission Candidates from Donor-Acceptor Copolymers [CC-026]**
Terence Blaskovits, EPFL Lausanne
M. Fumanal, S. Vela, C. Corminboeuf*

15:00 **Spin gap learning of carbenes with strongly correlated electrons [CC-027]**
Max Schwilk, University of Basel
D. N. Tahchieva, O. A. von Lilienfeld*

Chemistry and the Environment [EV]

Session Endowment:
Syngenta Crop Protection AG
Chairs: Prof. Kathrin Fenner, Eawag Dübendorf/University of Zurich
Prof. Tamar Kohn, EPFL Lausanne

10:00 **Organic Aerosol Composition: Effects on Health and Climate [EV-011]**
Markus Kalberer, University of Basel
J. Campbell, J. Zhang, K. Wolfer, B. Utinger, N. Bukowiecki, P. Gallimore, C. Giorio, I. Kourtchev

10:30 **Photochemical degradation of iron(III)-citrate/citric acid aerosol quantified with the combination of three complementary experimental techniques and a kinetic process model [EV-013]**
Jing Dou, ETH Zurich
P. A. Alpert, P. Corral Arroyo, B. Luo, T. Peter, M. Ammann, U. K. Krieger

10:45 **A decade of atmospheric CO_2 mole fraction and stable isotope ratios at Jungfraujoch measured by QCLAS, GC-FID and IRMS [EV-014]**
Simone Pieber, Empa, Dübendorf
B. Tuzson, S. Henne, U. Karstens, H. Moossen, A. Jordan, M. Rothe, D. Brunner, M. Steinbacher, L. Emmenegger*

11:00 **Plant and microbiota-dependent effects on arsenic behavior in the soil-plant system [EV-015]**
Hang Guan, University of Bern
V. Caggìa, M. Coll-Crespi, X. Liu, A. Mestrot, M. Dell'Aera, M. Bigalke

11:15 **Species-specific isotope tracking of mercury bioaccumulation and biotic transformations by natural pico-nanoplankton communities in a eutrophic lake [EV-016]**
Thibaut Cossart, University of Geneva
J. Garcia-Calleja, E. Tessier, K. Kavanagh, Z. Pedrero, V. Slaveykova*, D. Amouroux*

11:30 **Identity of the Cu(II) Active Site on Alumina for the Stepwise Selective Conversion of Methane to Methanol [EV-017]**
Jordan Meyet, ETH Zurich
A. Ashuiev, G. Noh, M. Newton, D. Klose, K. Searles, A. P. van Bavel, A. D. Horton, G. Jeschke, C. Copéret*, J. A. van Bokhoven*

13:30 **Crop protection in a changing climate [EV-021]**
Mathilde Lachia, Syngenta Crop Protection AG

14:00 **Exploring extracellular wastewater peptidases to inform the design of sustainable peptide-based antibiotics [EV-023]**
Michael Zumstein, Eawag, Dübendorf
D. Helbling, J. Werner, M. Zumstein*, K. Fenner*

14:15 **The relevance and role of "long-lived" photooxidants in aquatic organic photochemistry [EV-024]**
Stephanie C. Remke, Eawag/EPFL Lausanne
U. von Gunten, S. Canonica*

14:30 **Natural toxin mobility in soils – Mechanistic insights into multifunctional, ionizable organic compound sorption [EV-025]**
Carina D. Schönsee, Agroscope
F. E. Wettstein, T. D. Bucheli*

14:45 **Occurrence of pesticide residues in agricultural soils and their impact on indicators for soil life [EV-026]**
Judith Riedo, University of Zurich
F. Walder, T. D. Bucheli, M. G. van der Heijden*

15:00 **Environmentally conscious use of surfactant TPGS-750-M in water-based synthesis [EV-027]**
Christoph Krell, Novartis AG
F. Gallou, M. Parmentier

Inorganic & Coordination Chemistry [IC]

CASALE

Session Endowment: Casale SA
Chairs: Prof. Marinella Mazzanti, EPFL Lausanne
Prof. Kay Severin, EPFL Lausanne
Prof. Roger Alberto, University of Zurich

10:00 **Casale Strategy in ammonia synthesis: How to use engineering solutions to exploit the maximum benefits of the catalysts [IC-011]**
Pierdomenico Biasi, Casale SA
E. Filippi

10:30 **Synthesis and structural characterization of sodalite nanosheets and their films [IC-013]**
Mostapha Dakhchoune, EPFL Lausanne
K. V. Agrawal*

10:45 **Graphene nanoflake antibody conjugates for multimodal imaging [IC-014]**
Jennifer Lamb, University of Zurich
C. Salzmann, J. P. Holland*

11:00 **Alkali-Metal-Mediated Ferration (*AMM*Fe): Synthetic and Structural Studies with Fluoroarenes and Beyond [IC-015]**
Lewis C.H. Maddock, University of Bern
E. Hevia*

11:15 **From Water-stable Uranyl(V) to Uranium(IV) Polyoxometalates [IC-016]**
Radmila Faizova, EPFL Lausanne
L. Chatelain, R. Bernier-Latmani, A. Chauvin, F. Fadaei-Tirani, R. Scopelliti, M. Mazzanti*

11:30 **A Chiral $(NH)_2P_2$ Macrocylic Manganese(I) Catalyst for the Asymmetric Transfer Hydrogenation of Ketones [IC-017]**
Alessandro Passera, ETH Zurich
A. Mezzetti*

13:30 **Making, Breaking, and Elucidating Uranium-Nitrogen Multiple Bonds [IC-021]**
Suzanne Bart, Purdue University
T. S. Collins, E. Coughlin, M. Zeller

14:00 **Radiochemistry at PSI and the Chemistry of Transactinide Elements [IC-023]**
Patrick Steinegger, Paul Scherrer Institute (PSI), Villigen
P. Steinegger*

14:15 **The Atomic-Level Structure of Cementitious Calcium Aluminate Silicate Hydrate [IC-024]**
Pinelopi Moutzouri, EPFL Lausanne

14:30 **Two-gap to single-gap superconducting transition in the $Ca_{1-x}Sr_xAlSi$ Solid Solution [IC-025]**
Dorota I. Walicka, University of Zurich
Z. Guguchia, J. Lago, O. Blacque, R. Lefèvre, K. Ma, F. O. von Rohr*

14:45 **Silicon Oxycarbide as a Host Matrix of Choice to Stabilize Li-Ion Storage in Nanosized Alloying Elements [IC-026]**
Romain Dubey, ETH Zurich
P. Vallachira, F. Krumeich, G. Blugan, K. V. Kravchyk, T. Graule*, M. V. Kovalenko*

15:00 **Improvement of a Single-Ion Magnet Performance Using the Surface Organometallic Chemistry Approach [IC-027]**
Maciej Korzyński, ETH Zurich
Z. J. Berkson, O. Cador, B. Le Guennic, C. Copéret*

Medicinal Chemistry & Chemical Biology [MC]

Lonza

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

10:00 **SCS Division of Medicinal Chemistry & Chemical Biology: Activities 2020/21 and General Assembly 2020 [MC-011]**
Prof. J.-L. Reymond, DMCCB President/University of Bern

10:15 **Synthesis and biological investigation of new (–)-zampanolide analogues [MC-012]**
Simone Berardozzi, ETH Zurich
T. Brütsch, A. Prota, E. Cotter, E. Bonvin, J. Estevez Gallego, M. Steinmetz, J. F. Díaz Pareira, C. Steuer, K. Altmann*

10:30 **Mini-Monoplant Technology for Pharmaceutical Manufacturing [MC-013]**
Petteri Elsner, Lonza AG

10:45 **Synthesis and characterization of an adenosine A_1 receptor agonist with non-opioid analgesic properties based on Gα signaling bias [MC-014]**
Barbara Preti, University of Bern
M. Leuenberger, M. Lochner*

11:00 **Discovery and optimization of novel LpxC inhibitors for the treatment of serious Gram-negative infections [MC-015]**
Jean Surivet, Idorsia Pharmaceuticals Ltd.
P. Panchaud, G. Rueedi

11:15 **Human and Chimp CPEB3 ribozymes: unexpected fold of the HDV-like ribozymes [MC-016]**
Anna I. Przytula-Mally, University of Zurich
S. Engilberge, S. Johannsen, E. Freisinger, V. Olieric, R. K. Sigel*

11:30 **Discovery of Potent Selective $GABA_A$ Alpha5 Positive Allosteric Modulators (PAMs) for the treatment of neurological disorders [MC-017]**
Giuseppe Cecere, F. Hoffmann-La Roche AG

13:30 **The effects of chemical reactions on codon drift in DNA encoded libraries [MC-021]**
Basilius Sauter, University of Basel
L. Schneider, C. Stress, D. Gillingham*

13:45 **Microcycle: An Integrated Design-Make-Test-Analyse Platform to Accelerate Drug Discovery [MC-022]**
Alexander N. Marziale, Novartis Pharma AG

14:00 **Synthetic Collagen Heterotrimers by Conformational Design [MC-023]**
Nina B. Hentzen, ETH Zurich
V. Islami, H. Wennemers*

14:15 **Stepwise Design of γ-Secretase Modulators [MC-024]**
Rosa M. Rodríguez Sarmiento, F. Hoffmann-La Roche AG

14:30 **High-affinity glycomimetic ligands for human Siglec-8 [MC-025]**
Gabriele Conti, University of Basel
B. Kroezen, J. Cramer, B. Girardi, S. Rabbani, O. Schwardt, D. Ricklin, R. Pieters, B. Ernst*

14:45 **Target-based Identification and Optimization of Toll-like Receptor 7 and 8 Antagonists [MC-026]**
Thomas Knoepfel, Novartis Pharma AG
C. Betschart, R. Glatthar, E. Vangrevelinghe, T. Junt, S. Hawtin, J. Blank

15:00 **Immunological Epitope Mapping of the SARS-CoV-2 Spike Protein [MC-027]**
Lluc Farrera Soler, University of Geneva
S. Barluenga, J. Daguer, N. Winssinger*

Organic Chemistry [OC]

Session Endowment: Janssen R&D / Cilag AG

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

10:00 **Ring Expansion Approaches for the Synthesis of Functionalised Macrocycles [OC-011]**
William Unsworth, University of York

10:30 **Iridium-catalyzed acid-assisted asymmetric hydrogenation of oximes to hydroxylamines [OC-013]**
Josep Mas-Roselló, EPFL Lausanne
T. Smejkal, N. Cramer*

10:45 **Fluorescent Probes to Image Physical Forces in Living Cells [OC-014]**
Karolina Strakova, University of Geneva
J. López-Andarias, G. Licari, A. Colom, N. Jiménez-Rojo, E. Tajkhorshid, A. Roux, H. Riezman, N. Sakai, S. Matile*

11:00 **Assessment of the Synthetic Feasibility of Generated Chemical Space by Computer Assisted Synthesis Planning [OC-015]**
Amol Thakkar, University of Bern
V. Chadimova, E. J. Bjerrum, O. Engkvist, J. L. Reymond*

11:15 **Synthesis of Tetraarylethene Luminogens by C-H Vinylation of Arenes [OC-016]**
Abdusalom Suleymanov, EPFL Lausanne
K. Severin*

11:30 **Divergent Total Synthesis of (–)-epicoccin G and (–)-rostratin A Enabled by Double C(sp^3)–H Activation [OC-017]**
Pierre Thesmar, University of Basel
O. Baudoin*

13:30 **Recent Case Study by Janssen R&D [OC-021]**
Simon Wagschal, Janssen Pharmaceutica

14:00 **Understanding Catalysis in Iron Heme Metalloproteins Using Non-Canonical Amino Acids [OC-023]**
Matthias Tinzl, ETH Zurich
T. Hayashi, M. Pott, U. Krengel, J. Proppe, J. Soetbeer, D. Klose, M. Reiher, G. Jeschke, D. Hilvert*

14:15 **Radical Functionalization of Cyclopropenes for the Synthesis of Bicyclo[3.1.0]hexanes and Substituted Alkenes [OC-024]**
Bastian Muriel, EPFL Lausanne
A. Gagnebin, J. Waser*

14:30 **A multi-modality platform to develop supramolecular radiopharmaceuticals [OC-025]**
Faustine D'Orchymont, University of Zurich
J. P. Holland*

14:45 **Synthesis of chiral and redox-active covalent organic cages [OC-026]**
Hsin-Hua Huang, University of Basel
T. Šolomek*

15:00 **Polar Opposites in Phosphorus Catalysis: Applications of 1,3,2-Diazaphospholenes [OC-027]**
John Reed, EPFL Lausanne
N. Cramer*

Physical Chemistry [PC]

Session Endowment: Carl ZEISS AG

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

10:00 **Unravelling the intricate interplay between donor and acceptor materials in bulk heterojunction blends for organic photovoltaics [PC-011]**
Sabine Van Doorslaer, University of Antwerp
I. Sudakov, M. Van Landeghem, W. Maes, E. Goovaerts

10:30 **A Supramolecular Approach to Hybrid Perovskite Photovoltaics [PC-013]**
Jovana Milic, EPFL Lausanne
M. A. Ruiz-Preciado, D. J. Kubicki, A. Hofstetter, L. Emsley*, M. Graetzel*

10:45 **Size-selection: An essential step for understanding lead halide perovskite quantum optics [PC-014]**
Franziska Krieg, ETH Zurich
M. V. Kovalenko

11:00 **Electronegativity and Location of Anionic Ligands Drive Yttrium NMR for Molecular, Surface and Solid-State Structures [PC-015]**
Lukas Lätsch, ETH Zurich
E. Lam, C. Copéret*

11:15 **Quantifying interface diffusion in Li ion battery cathode materials [PC-016]**
Peter Benedek, ETH Zurich
O. K. Forslund, E. Nocerino, N. Yazdani, N. Matsubara, Y. Sassa, M. Medarde, M. Månsson, V. Wood*

11:30 **Surface Potential and Interfacial Water Order at the Amorphous TiO_2 Nanoparticle/Aqueous Interface [PC-017]**
Marie Bischoff, EPFL Lausanne
D. Biriukov, M. Předota, S. Roke*, A. Stucki*

13:30 **LSM 9 Family – Versatile Confocal Microscopy for Advanced Imaging and Surface Topography [PC-021]**
Christine Strasser, Carl ZEISS AG

14:00 **Towards in-cell drug detection and quantification by MAS DNP [PC-023]**
Andrea Bertarello, EPFL Lausanne
L. Emsley*

14:15 **Interchromophore conformation and geometrical flexibility governs the fate of triplet pairs generated by singlet fission [PC-024]**
Alexander Aster, University of Geneva
F. Zinna, C. Rumble, J. Lacour, E. Vauthey*

14:30 **Unravelling the Mechanism of Ultrafast Intrinsic Charge Generation in Cyanine Dyes [PC-025]**
George Fish, EPFL Lausanne
J. Moreno Naranjo, E. Hack, A. Billion, I. Krossing, F. Nüesch, J. Moser*

14:45 **Precision Spectroscopy, Coherent Manipulation and State-to-State Chemistry of Single Molecular Ions [PC-026]**
Mudit Sinhal, University of Basel
Z. Meir, A. Shlykov, M. F. Roguski, S. Willitsch*

15:00 **Chiral control of spin-crossover dynamics in Fe(II) complexes [PC-027]**
Malte Oppermann, EPFL Lausanne
F. Zinna, J. Lacour, M. Oppermann*, M. Chergui*

Polymers, Colloids & Interfaces [PI]

Session Endowment: Dow Europe
Chairs: Prof. Walter Caseri, ETH Zurich
Dr. Dominik Brühwiler, ZHAW Wädenswil

10:00 **Novel hyperbranched organofunctional polyalkoxysiloxanes: versatile precursors for molecular-level design of advanced colloidal materials [PI-011]**
Matthias Koebel, Empa, Dübendorf
A. Stojanovic, W. J. Malfait, A. Nour, L. Huber

10:30 **Mass transport studies in porous silica as a function of core-shell architecture [PI-013]**
Samuel Gallagher, ZHAW Wädenswil
P. Schlauri, E. Cesari, J. Durrer, D. Brühwiler*

10:45 **Functionalization of Chitosan for Non-viral Gene Delivery to the Liver [PI-014]**
Laura Nicolle, EPFL Lausanne
C. Journot, J. Casper, P. Detampel, T. Einfalt, H. Grisch-Chan, B. Thöny, J. Huwyler, S. Gerber-Lemaire*

11:00 **Supramolecular Assembly of Amphiphilic DNA into Vesicular Architectures [PI-015]**
Simon Rothenbühler, University of Bern
I. Iacovache, S. M. Langenegger, B. Zuber, R. Häner*

11:15 **Quantitative mechanochromism of polydiacetylenes at the nanoscale [PI-016]**
Levente Juhasz, University of Geneva
R. D. Ortuso, K. Sugihara*

11:30 **Patience is a Virtue: Self-Assembly and Physico-Chemical Properties of Cellulose Nanocrystal Allomorphs [PI-017]**
Gwendoline Delepierre, University of Fribourg, Adolphe Merkle Institute
W. Thielemans, S. Eyley, C. Weder, E. Cranston*, J. Zoppe*

13:30 **Functionalized Polyolefins for Recycling & Dow's Sustainability Commitments [PI-021]**
Olaf Henschke, Dow Europe GmbH
K. Hausmann, I. Arroyo

14:00 **Polymersome clusters for advanced nanotheranostics [PI-023]**
Claire Meyer, University of Basel
J. Liu, I. Craciun, D. Wu, H. Wang, M. Xie, M. Fussenegger, C. G. Palivan*

14:15 **Signaling Deformation in Polymeric Materials *via* Supramolecular Interactions [PI-024]**
Derek Kiebala, University of Fribourg, Adolphe Merkle Institute
S. Schrettl, C. Weder*

14:30 **Simultaneous extraction and controlled chemical modification of polymeric lignin from hardwood [PI-025]**
Stefania Bertella, EPFL Lausanne
J. Luterbacher*

14:45 **Ligand-Assisted Solid Phase Synthesis of Mixed-Halide Perovskite Nanocrystals for Highly Electroluminescent Light-Emitting Diodes [PI-026]**
Simon Solari, ETH Zurich
S. Kumar, J. Jagielski, N. M. Kubo, F. Krumeich, C. Shih*

15:00 **Alginate-based hydrogels as multifunctional materials for cell transplantation, and production of microspheres with a microfluidic technique [PI-027]**
Luca Szabo, EPFL Lausanne
S. Gerber-Lemaire*

VIRTUAL POSTER SESSIONS (SHORT VIDEOS)

Poster Presentation Title [Code]
Fist line = Presenting Author, Affiliation
Second line = Co-authors
* Research Head(s)

Analytical Sciences [AS] Virtual Poster Session

Using SLIM-based IMS-IMS together with cryogenic infrared spectroscopy for glycan analysis [AS-101]
Priyanka Bansal, EPFL Lausanne
V. Yatsyna, A. Abi Khordr, S. Warnke, A. Ben Faleh, N. Yalovenko, V. Wysocki, T. R. Rizzo*

Tip-Enhanced Raman Spectroscopy of Biologically Relevant Membranes [AS-102]
Giovanni Luca Bartolomeo, ETH Zurich
G. Goubert, R. Zenobi*

Linking paper-based analytics to ambient mass spectrometry for trace analysis of environmental toxins [AS-103]
Alina I. Begley, ETH Zurich
Y. Lai, R. Zenobi*

Gas-phase fragmentation of β-cyclodextrin [AS-104]
Pia S. Bruni, University of Bern
S. Schürch*

Exploring Dialysis Membranes as Liquid Junction Materials [AS-106]
Tara Forrest, University of Geneva
E. R. Heller*

Improvements on the depth profiling performance of a miniature LIMS system using double-pulse laser irradiation [AS-107]
Valentine Grimaudo, University of Bern
A. Riedo, M. Tulej, R. Lukmanov, N. F. Ligterink, P. Wurz*

NEXAFS without a Tunable X-ray Source: Signal Reconstruction by means of Compressive Sensing [AS-108]
Yousuf Hemani, Empa, Dübendorf/University of Zurich
D. Bleiner*

Tracking Isomers in Breath Metabolomics by Coupling Gas Chromatography with Secondary Electrospray Ionization Mass Spectrometry [AS-109]
Jérôme Kaeslin, ETH Zurich
T. Bruderer, R. Zenobi*

Characterization of nanoparticles in organic matrices by means of Single-Particle Inductively Coupled Plasma Mass Spectrometry [AS-110]
Jovana Kocic, ETH Zurich
D. Günther, B. Hattendorf*

Listening with curiosity – Tracking the acoustic response of portable LA [AS-111]
Stefan Kradolfer, ETH Zurich
K. Heutschi, J. Koch, D. Günther*

Accurate and Precise stoichiometric Tuning of the Li/Mn ratio in $LiMn_2O_4$ Thin Films using Laser Ablation [AS-112]
Kevin Kraft, Empa, Dübendorf/University of Zurich
C. Wyder, N. Ohannessian, M. Trottmann, A. Wichser, D. Bleiner*, T. Lippert*

Monitoring peppermint washout in the breath metabolome by secondary electrospray ionization-high resolution mass spectrometry [AS-113]
Jiayi Lan, ETH Zurich
R. Zenobi*

Exploring the High Mass Limits of Ionization with a DBDI Source [AS-114]
Qi Liu, EPFL Lausanne
R. Zenobi*

Tip-enhanced Raman Spectroscopy on Two-Dimensional Polymers [AS-115]
Timo S.G. Niepel, ETH Zurich
W. Wang, A. Schlüter, R. Zenobi*

Thermal Denaturation of RNAse A Bound to a Library of DNA/RNA Ligands: Binding Constants and Thermodynamic Analysis of Multiple Stable Intermediates Revealed by Electrospray Mass Spectrometry with a Temperature-Controlled Source [AS-116]
Irina Oganesyan, ETH Zurich
A. Marchand, R. Zenobi*

Thermodynamic Studies of DNA G-quadruplexes and Characterization of a GQ-Specific Antibody Using Temperature-Controlled nanoESI MS [AS-117]
Adam Pruška, ETH Zurich
D. Böken, A. Marchand, R. Zenobi*

Deep UV Raman for in situ detecting of water contaminants [AS-118]
Andrea Sterzi, Empa, Dübendorf
U. Schneider, O. Sambalova, R. Figi, D. Bleiner, A. Borgschulte*

Standardization Procedure for Breath Analysis by Secondary Electrospray Ionization Mass Spectrometry [AS-119]
Bettina Streckenbach, ETH Zurich
J. Sakas, S. Mueller, N. Perkins, A. Moeller, M. Kohler, R. Zenobi*

Visualization of volatile intermediates in the course of CO_2 methanation over a commercial nickel on alumina/silica catalyst by DRIFTS and INS [AS-120]
Jasmin Terreni, Empa, Dübendorf/University of Zurich
O. Sambalova, S. Rudic, S. F. Parker, A. J. Ramirez-Cuesta, A. Borgschulte*

Progress in the development of a sample introduction system for the downwards-pointing vertical ICPMS for future particle and cell analysis [AS-121]
Thomas Vonderach, ETH Zurich
B. Hattendorf, D. Günther*

Catalysis Sciences & Engineering [CE] Virtual Poster Session

Copper-Gallium Alloy Structure Determines Promotional Effect of Gallium in the CO_2 Hydrogenation to Methanol [CE-101]
Jan L. Alfke, ETH Zurich
C. Copéret*, O. V. Safonova*

Formation and dynamics of copper-oxo species in zeolites evaluated using oxygen-18 isotope exchange and oxidation kinetics [CE-102]
Mikalai Artsiusheuski, ETH Zurich
J. A. van Bokhoven, V. Sushkevich*

Thermal degradation of UiO-66: Glass formation [CE-103]
Muhammad Athar, Paul Scherrer Institute (PSI), Villigen/ETH Zurich
R. Przemyslaw, J. A. van Bokhoven*, M. Ranocchiari*

Etched Nickel Foam as promising Catalyst for Overall Water Splitting [CE-104]
S. E. Balaghi, University of Zurich
G. R. Patzke*

Introducing Lewis acidity in zeolites by Ion-Exchanging Extra-Framework Cations [CE-105]
Syeda R. Batool, ETH Zurich
V. Sushkevich, F. Krumeich, M. Ravi, R. Przemyslaw, J. A. van Bokhoven*

Low-Temperature Activity and Initiation of Reduced Supported Mo and W Olefin Metathesis Catalysts [CE-106]
Zachariah Berkson, ETH Zurich
L. Lätsch, K. Chan, C. Copéret*

Hydride Catalysis [CE-107]
Emanuel Billeter, Empa, Dübendorf/University of Zurich
A. Borgschulte*

Silica-supported cobalt for the heterogeneous aerobic oxidation of methane to a methyl-derivative [CE-108]
Andrea Blankenship, ETH Zurich
M. Ravi, J. A. van Bokhoven*

Carrier induced modification of palladium nanoparticles on porous boron nitride for selective alkyne hydrogenation [CE-109]
Simon Büchele, ETH Zurich
E. Fako, F. Krumeich, R. Hauert, O. V. Safonova, N. López, S. Mitchell, J. Pérez-Ramírez*

Fe-FER catalyst for nitrous oxide abatement in simulated feeds of nitric acid plant [CE-110]
Filippo Buttignol, Paul Scherrer Institute (PSI), Villigen
A. Garbujo, R. Lanza, P. Biasi, O. Kröcher*, D. Ferri*

Defective UiO-66 and its interaction with solvents, acids and bases [CE-111]
Daniele Cartagenova, Paul Scherrer Institute (PSI), Villigen/ETH Zurich
F. A. Peixoto Esteves, N. T. Fischer, J. A. van Bokhoven, M. Ranocchiari*
V. Yatsyna, A. Abi Khordr, S. Warnke, A. Ben Faleh, N. Yalovenko, V. Wysocki, T.

Assessment of the impact of mesopore geometry in hierarchical MFI zeolites on the performance in methanol to olefins by hysteresis scanning [CE-112]
Alessia Cesarini, ETH Zurich
B. Puértolas, S. Mitchell, J. Kenvin, J. Pérez-Ramírez*

Time-resolved XAS study of the formation of cobalt hydride intermediates of cobaloxime catalyst during photoinduced pH jump [CE-113]
Jingfeng Chen, Paul Scherrer Institute (PSI), Villigen
M. Nachtegaal, E. Fabbri, T. J. Schmidt*, G. Smolentsev*

Design and Evolution of Chimeric Streptavidin for protein-directed Dual Gold Catalysis [CE-114]
Fadri Christoffel, University of Basel
N. V. Igareta, T. R. Ward*

In-situ investigations of spillover over molybdenum-based catalysts [CE-115]
Claudiu Colbea, ETH Zurich
J. A. van Bokhoven*, M. G. Willinger*

Molecular-Level Insight in Supported Olefin Metathesis Catalysts by Combining Surface Organometallic Chemistry, High Throughput Experimentation, and Data Analysis [CE-116]
Jordan De Jesus Silva, ETH Zurich
A. Fedorov, M. A. Ferreira, M. S. Sigman, C. Copéret*

Structure and reactivity of low-nuclearity iron-based catalysts on carbon nitride for alkyne semi-hydrogenation [CE-117]
Dario Faust Akl, ETH Zurich
E. Vorobyeva, R. Hauert, F. Krumeich, D. Klose, O. V. Safonova, S. Mitchell, J. Pérez-Ramírez*

Windowless *in situ* imaging at increased pressure: Perforated MEMS chips in an ETEM [CE-118]
Hannes Frey, ETH Zurich
X. Huang, T. Sasaki, J. A. van Bokhoven*, M. G. Willinger*

Structure–adsorption relationship in metal-organic frameworks revealed by molar surface area and molar adsorption capacity [CE-119]
Patrick Gäumann, Paul Scherrer Institute (PSI), Villigen, ETH Zurich
F. A. Peixoto Esteves, D. Cartagenova, J. A. van Bokhoven, M. Ranocchiari*

Platinum single-atom catalysts for sustainable vinyl chloride production [CE-120]
Selina K. Kaiser, ETH Zurich
E. Fako, G. Manzocchi, F. Krumeich, A. H. Clark, R. Hauert, O. V. Safonova, N. López, J. Pérez-Ramírez*

Na K-edge XANES combined with ^{23}Na-NMR unravel structure–property relationships in Na_2CO_3-promoted CaO-based sorbents for CO_2 capture [CE-121]
Maximilian Krödel, ETH Zurich
M. Nadjafi, F. Donat, A. H. Bork, P. M. Abdala*, C. R. Müller*

Role of Water on the Structure of Palladium for Complete Oxidation of Methane [CE-122]
Xiansheng Li, ETH Zurich
J. A. van Bokhoven, L. Artiglia

Dynamic semiconductor-electrolyte interfaces during photoelectrochemical water oxidation [CE-123]
Jingguo Li, University of Zurich
G. R. Patzke*

Operando Spectroelectrochemical Observation of Surface States and Active Sites in Chalcopyrite Photocathodes for Solar Water Reduction [CE-124]
Yongpeng Liu, EPFL Lausanne
K. Sivula*, N. Guijarro*

Hybridization of Fossil and CO_2-Based Routes for Ethylene Production using Renewable Energy [CE-125]
Antonio Martín, ETH Zurich
I. Ioannou, S. C. D'Angelo, J. Pérez-Ramírez*, G. Guillén-Gosálbez*

Revealing the dynamics of Sabatier reaction by IR thermography [CE-126]
Emanuele Moioli, Paul Scherrer Institute (PSI), Villigen
R. Mutschler, A. Züttel*

Efficient membrane-based solutions for increasing sustainability of processes in fine chemical and pharmaceuticals industry [CE-127]
Marzio Monagheddu, VITO – Flemish Institute of Technology
D. Ormerod, F. Nahra, A. Buekenhoudt

Defect-induced activity enhancement in Ce-substituted lanthanum strontium manganites for solar thermochemical CO_2 splitting [CE-128]
J. M. Naik, University of Zurich
B. Bulfin, A. Steinfeld, G. R. Patzke*

Revealing the Reaction Mechanism of Benzenediols in Catalytic Pyrolysis Using HZSM-5 [CE-129]
Zeyou Pan, Paul Scherrer Institute (PSI), Villigen
A. Puente-Urbina, A. Bodi, J. A. van Bokhoven*, P. Hemberger*

Bifunctional catalysts for coke hydrogenolysis in methanol-to-hydrocarbons processes [CE-130]
Vladimir Paunović, Paul Scherrer Institute (PSI), Villigen
V. Paunović, J. A. van Bokhoven*

Multiscale First-Principles Calculations of Propane Dehydrogenation on PtGa Nanoparticles Supported on Ga-Doped Silica [CE-131]
Pierre A. Payard, ETH Zurich
L. Rochlitz, L. Foppas, K. Searles, B. Leuthold, A. Coma-Vives, C. Copéret*

Catalyst design for direct CO_2 hydrogenation to transportation fuels [CE-132]
Eva Perković, ETH Zurich
C. Mondelli, J. Pérez-Ramírez*

Impact of mixed CO_2-CO feeds on methanol synthesis over In_2O_3-based catalysts [CE-133]
Thaylan Pinheiro Araújo, ETH Zurich
C. Mondelli, J. A. Stewart, J. Pérez-Ramírez*

On the mechanism of methane conversion in non-oxidative conditions [CE-134]
Allen Puente-Urbina, ETH Zurich
Z. Pan, V. Paunović, P. Šot, P. Hemberger, J. A. van Bokhoven*

The Impact of Preparative History and Driving Force on the Water Oxidation Activity of Spinel-Type Cobalt Oxide [CE-135]
Lukas Reith, University of Zurich
K. Lienau, C. A. Triana, S. Siol, G. R. Patzke*

Crystallographic and morphological optimization of catalytic copper foil for hydrogen-sieving single-layer graphene membranes [CE-136]
Mojtaba Rezaei, EPFL Lausanne
K. V. Agrawal*

Heterogeneous, Bimetallic Pt-based Catalysts for Propane Dehydrogenation via Surface Organometallic Chemistry [CE-137]
Lukas Rochlitz, ETH Zurich
C. Copéret*

Beneficial effect of steam reforming of CH_4 on NO removal on a three-way catalyst under transient conditions [CE-138]
Maneka Roger, Paul Scherrer Institute (PSI), Villigen
D. Ferri, O. Kröcher*

Beneficial effect of steam reforming of CH_4 on NO removal on a three-way catalyst under transient conditions [CE-139]
Maneka Roger, Paul Scherrer Institute (PSI), Villigen
D. Ferri, O. Kröcher*

Anomalous X-ray diffraction at the Al and Si K-edges [CE-140]
Przemyslaw Rzepka, ETH Zurich
A. Pinar, T. Huthwelker, A. Knorpp, L. McCusker, C. Baerlocher, J. A. van Bokhoven

Performance of metal-catalyzed hydrodebromination of dibromomethane analyzed by descriptors derived from statistical learning [CE-141]
Ali Saadun, ETH Zurich
S. Pablo-Garcia, V. Paunović, Q. Li, A. Sabadell-Rendón, K. Kleemann, F. Krumeich, N. López, J. Pérez-Ramírez*

NHCAuOTf Catalyzed Alkyne Hydration Under Mild Reaction Conditions [CE-142]
Irene Sacco, University of Bern
M. Albrecht*, F. Paradisi*

Operando quick XAS of oxygen activation mechanism over supported bimetallic Pt-Fe catalysts [CE-143]
Ilia Sadykov, Paul Scherrer Institute (PSI), Villigen
A. H. Clark, J. A. van Bokhoven, M. Nachtegaal, O. V. Safonova*

Magnetic field effect on the electrochemical hydrogen evolution reaction with ferromagnetic electrodes [CE-144]
Olga Sambalova, Empa, Dübendorf/University of Zurich
E. Billeter, O. Yildirim, A. Sterzi, D. Bleiner, A. Borgschulte*

Nanostructure Engineering for Heterogeneous Catalysis [CE-145]
Louisa Savereide, EPFL Lausanne
B. P. Le Monnier, J. Luterbacher*

Formation of iron(II) single sites on the surface of silica and their role in the transformation of methane to higher hydrocarbons [CE-146]
Petr Šot, ETH Zurich
M. Newton, A. P. van Bavel, A. D. Horton, C. Copéret*, J. A. van Bokhoven*

***Operando* X-Ray Absorption Spectroscopy Identifies Monoclinic ZrO_2: In Solid Solution as the Active Phase for the Hydrogenation of CO_2 to Methanol [CE-147]**
Athanasia Tsoukalou, University of Bern
A. Armutlulu, E. Willinger, C. R. Müller, P. M. Abdala*, A. Fedorov*

Laser-microstructured copper reveals selectivity patterns in the electrocatalytic reduction of CO_2 [CE-148]
Florentine Veenstra, ETH Zurich
N. Ackerl, A. J. Martín, J. Pérez-Ramírez*

Electron diffraction resolves the aluminium sites in a zeolite catalyst [CE-149]
Julian Wennmacher, Paul Scherrer Institute (PSI), Villigen
P. Rzpeka, T. Li, E. Fröjd, B. Schmitt, J. A. van Bokhoven*, T. Gruene*

Dynamics of catalyst structure resolved on an atomic scale by in situ electron diffraction [CE-150]
Julian Wennmacher, Paul Scherrer Institute (PSI), Villigen
A. J. Knorpp, H. Frey, T. Gruene, J. A. van Bokhoven*, M. G. Willinger*

Graphene conjugated single site catalysts for high performance electrocatalytic water oxidation [CE-151]
Wenchao Wan, University of Zurich
Y. Zhao, C. A. Triana, G. R. Patzke*

Self-Templating Strategies for Transition Metal Sulfide Nanoboxes as Robust Bifunctional Electrocatalysts [CE-152]
Yonggui Zhao, University of Zurich
C. K. Mavrokefalos, G. R. Patzke*

Mechanistic insights into catalyzed propane oxychlorination by *operando* EPR spectroscopy [CE-153]
Guido Zichittella, ETH Zurich
Y. Polyhach, G. Jeschke*, J. Pérez-Ramírez*

Computational and Theoretical Chemistry [CC] Virtual Poster Session

Quantum Dynamics with the Time-Dependent Density Matrix Renormalization Group [CC-101]
Alberto Baiardi, ETH Zurich
M. Reiher*

Real-Time Spectroscopy for an Interactive Quantum Chemistry Framework [CC-102]
Francesco Bosia, ETH Zurich
T. Weymuth, S. Polonius, M. Reiher*

A time-reversible integrator for the time-dependent Schrödinger equation on an adaptive grid [CC-104]
Seonghoon Choi, EPFL Lausanne
J. Vaníček*

The Role of Substrate Binding in the O_2 Activation Pathway of Naphthalene 1,2-Dioxygenase [CC-105]
Katja S. Csizi, ETH Zurich
L. Eckert, C. Brunken, M. Reiher*, T. B. Hofstetter*

Advanced Data-Driven Manufacturing using Autoencoders [CC-106]
Théophile Gaudin, IBM Research Europe
O. Schilter, F. Zipoli, T. Laino

Electric Field Gradient calculation within Frozen-Density Embedding Theory [CC-107]
Yann Gimbal-Zofka, University of Geneva
M. Fu, N. Ricardi, C. E. Gonzalez, T. A. Wesolowski*

On-the-fly ab initio semiclassical evaluation of electronic coherences in polyatomic molecules reveals a simple mechanism of decoherence [CC-108]
Nikolay Golubev, EPFL Lausanne
T. Begušić, J. Vaníček

Identifying and Designing Ligand Fields by Computational Alchemy [CC-109]
Christopher P. Gordon, ETH Zurich
C. Copéret*

Automated Chemical Reaction Space Exploration of a Proton Reduction Mechanism [CC-110]
Stephanie Grimmel, ETH Zurich
M. Reiher*

Complete active space analysis of a reaction pathway: investigation of the oxygen-oxygen bond formation[1] [CC-111]
Ruocheng Han, University of Zurich
S. Luber*

Excited-state properties for semi-empirical tight binding [CC-112]
Anna Hehn, University of Zurich
F. Belleflamme, J. Hutter*

Quantum tunnelling in electron-transfer reactions [CC-113]
Eric Heller, ETH Zurich
J. O. Richardson*

Quantum Tunnelling in Isotopically-Substituted Systems with Machine Learning and Ab Initio Instanton Theory [CC-114]
Gabriel Laude, ETH Zurich
E. M. Jahr, J. O. Richardson*

Spin-mapping approach to nonadiabatic molecular dynamics [CC-115]
Johan Runeson, ETH Zurich
J. O. Richardson*

Nonadiabatic effects in electronic spectroscopy: a novel quantum-classical approach [CC-116]
Jonathan Mannouch, ETH Zurich
J. O. Richardson*

Extending spectroscopic applications of real time propagation [CC-117]
Johann Mattiat, University of Zurich
S. Luber*

Reliability of Tailored Coupled Cluster in Different Correlation Regimes [CC-118]
Maximilian Mörchen, ETH Zurich
L. Freitag, M. Reiher*

Frozen Density Embedding Theory exploiting experiment-derived densities for the environment [CC-119]
Niccolò Ricardi, University of Geneva
M. Ernst, T. A. Wesolowski*, P. Macchi*

Towards Spatially Sensitive Infrared Probes [CC-120]
Seyedeh Maryam Salehi, University of Basel

Molecular dynamics simulations to understand conformational behavior of cyclic peptides at polar/apolar interfaces [CC-121]
Christian Schellhaas, ETH Zurich
S. M. Linker, S. Riniker*

Chemical Reaction Grammar as Seen by Neural Networks: Unsupervised Attention-guided Atom-Mapping [CC-122]
Philippe Schwaller, IBM Research Europe
B. Hoover, J. L. Reymond, H. Strobelt, T. Laino*

Benchmarking Tight-Binding Predictions for Metal-Organic Frameworks [CC-123]
Beliz Sertcan, University of Zurich
A. Hehn, J. Hutter*

The effects of van der Waals dispersion corrections on the study of carbon nitrides membranes performance [CC-124]
Mohammad Tohidi Vahdat, EPFL Lausanne
D. Campi, N. Marzari*, K. V. Agrawal*

Unassisted Noise-Reduction of Chemical Reactions Data Sets [CC-125]
Alessandra Toniato, IBM Research Europe
P. Schwaller, A. Cardinale, J. Geluykens, T. Laino*

Nonadiabatic Instanton Rate Theory – Quantum Tunnelling beyond the Born-Oppenheimer Approximation [CC-126]
Rhiannon Zarotiadis, ETH Zurich
J. O. Richardson*

Chemistry and the Environment [EV] Virtual Poster Session

On the Real Aging of Diesel Oxidation Catalyst [EV-101]
Miren Agote-Aran, Paul Scherrer Institute (PSI), Villigen
C. Coffano, M. Elsener, F. Krumeich, O. Kröcher, D. Ferri*

Product Generation and Imaging of Photoactive and Viscous Organic Aerosol Particles [EV-102]
Peter Alpert, Paul Scherrer Institute (PSI), Villigen
J. Dou, U. K. Krieger, T. Peter, P. Corral Arroyo, S. Bjelic, D. Salionov, P. A. Alpert*, M. Ammann*

Plant protection products in soils: Determination of bioavailability by means of passive samples [EV-103]
Nora Bartolomé, Agroscope
J. Riedo, D. Wächter, T. D. Bucheli*

Unraveling Enzyme Kinetics of Organic Contaminant Oxygenations with the use of Kinetic Isotope Effects [EV-104]
Charlotte Bopp, Eawag, Dübendorf
S. G. Pati, H. E. Kohler, T. B. Hofstetter*

Photochemistry of organic matter in the atmosphere and its effect on mixed-phase cloud formation [EV-105]
Nadine Borduas-Dedekind, ETH Zurich
S. Müller, S. Bogler, N. Borduas-Dedekind*

Monitoring of priority substances in sediments of Switzerland [EV-106]
Carmen Casado-Martinez, Swiss Centre for Applied Ecotoxicology
S. Valsecchi, P. A. Lara-Martin, P. Marchand, F. Breider, Y. Schindler-Windhaber , B. J. Ferrari, I. Werner

The role of surface states on reduced TiO_2@$BiVO_4$ photoanodes: Enhanced water oxidation performance through improved electron transfer [EV-108]
Hang Chen, University of Zurich
J. Li, G. R. Patzke*

Bioaccumulation and transformation of mercury compounds by model phytoplankton: focus on green algae and cyanobacteria [EV-109]
Thibaut Cossart, University of Geneva
J. P. Santos, J. Garcia-Calleja, I. Worms, E. Tessier, L. Ouerdane, Z. Pedrero, V. Slaveykova*, D. Amouroux*

Transgenerational Fate of Polychlorinated Biphenyls from Cow to Calf during Gestation and Lactation [EV-110]
Charlotte Driesen, Empa, Dübendorf
R. Siegenthaler, M. Zennegg*, S. Lerch*

Exposure assessment of pyrrolizidine alkaloids in Swiss surface water combining retrospective data analysis and particular invasive *Senecio* monitoring [EV-111]
Barbara F. Günthardt, Agroscope
J. Hollender, H. Singer, M. Scheringer, T. D. Bucheli*

Application of *in vitro – in vivo* extrapolation to predict the bioaccumulation potential of fragrance chemicals [EV-112]
Lu Hostettler, Givaudan Schweiz AG
A. Natsch, G. Sanders, K. Jenner, H. Laue*

Quantification of Oxidant-Reactive Carbonous Sites in Dissolved Organic Matter [EV-113]
Joanna Houska, Eawag, Dübendorf
U. von Gunten*

Automated method to analyse cyanobacterial toxins and secondary metabolites in Swiss surface waters by online SPE-LC-HRMS/MS [EV-114]
Martin Jones, Eawag, Dübendorf
J. Bosshard, E. M. Janssen*

Mineral respiration of *Geobacter sulfurreducens* [EV-115]
Maksym Karamash, University of Fribourg
B. Giese*, B. M. Fromm*

Transformation of chlorinated paraffins by the bacterial dehalogenase LinB – Identification of hydroxylated metabolites [EV-116]
Marco C. Knobloch, Empa, Dübendorf/University of Zurich
L. Schinkel, I. Schilling, H. E. Kohler, P. Lienemann, D. Bleiner, N. Heeb*

Current Trends and Future Challenges of Rechargeable Aluminum-Graphite and Other Dual-Ion Batteries [EV-117]
Kostiantyn Kravchyk, ETH Zurich
M. V. Kovalenko

Reactions of nitrogen-containing compounds with ozone: kinetics and mechanisms [EV-118]
Sungeun Lim, Eawag, Dübendorf
C. S. McArdell, U. von Gunten*

Development of a Unified UHPLC-QTOF-MS Method for Benzoxazinoids Analysis [EV-119]
Pierre Mateo, University of Bern
J. D. Berset, M. Erb*, C. A. Robert*

Non-destructive method based on infrared spectroscopy and partial least square regression for the quantification of the ionic component of atmospheric particulate matter [EV-120]
Ugo Molteni, University of Milan
A. Piazzalunga, P. Fermo*

Towards Incorporation of Minor Elements in synthetic C-S-H [EV-121]
Anna Morales-Melgares, EPFL Lausanne
P. Moutzouri, P. Bowen, K. Scrivener*, L. Emsley*

Singlet oxygen quantum yields in environmental waters: critical evaluation of measurement techniques [EV-122]
Rachele Ossola, ETH Zurich
O. M. Jönsson, K. J. Moor, K. McNeill*

Wavelength dependence of singlet oxygen quantum yields from dissolved organic matter [EV-123]
Sarah Partanen, ETH Zurich
P. R. Erickson, D. E. Latch, K. McNeill*, K. J. Moor*

Occurrence of natural estrogens in surface waters of a catchment with intensive livestock farming in Switzerland [EV-124]
Daniela Rechsteiner, Agroscope
F. E. Wettstein, B. P. Warren, E. L. Vermeirssen, E. Simon, M. K. Schneider, J. Hollender, T. D. Bucheli*

First Halogenated Greenhouse Gas Measurements at the Beromünster Tall Tower in Switzerland [EV-125]
Dominique Rust, Empa, Dübendorf
M. K. Vollmer, M. Hill, P. Schlauri, S. Henne, I. Katharopoulos, L. Emmenegger, R. Zenobi, S. Reimann*

The role of diatom *Cyclotella meneghiniana* in aquatic Hg species transformations [EV-126]
João P. Santos, University of Geneva
T. Cossart, J. Garcia-Calleja, E. Tessier, D. Amouroux, V. Slaveykova*

Regulatory persistence assessment in water-sediment systems: Evaluating biotic and abiotic transformation of micropollutants [EV-127]
Carolin Seller, Eawag, Dübendorf
M. Honti, K. Fenner*

Dissolved organic matter as a modifier of Hg bioavailability to phytoplankton [EV-128]
Vera Slaveykova, University of Geneva
N. Regier, E. Moulin, K. Kavanagh , I. Worms

Dating the recent past. Chronometric potential of Si-32 – Part 1: Chemical separation and preparation in a pure state [EV-129]
Mario Veicht, Paul Scherrer Institute (PSI), Villigen/EPFL Lausanne
I. Mihalcea, P. Sprung, A. Pautz, C. Bailat, Y. Nedjadi, K. Kossert, C. Vockenhuber, A. Wallner, D. Schumann*

Inorganic & Coordination Chemistry [IC] Virtual Poster Session

Nuclear Quadrupole Resonance of multinary $FA_{1-x}Cs_xPbI_{3-y}Br_y$ Perovskites [IC-101]
Marcel Aebli, ETH Zurich
M. V. Kovalenko*

Alkoxide-Mediated Metal Halogen Exchange Reactions [IC-103]
Leonie J. Bole, University of Bern
N. R. Judge, E. Hevia*

The origin of trap-states in monodisperse formamidinium tin iodide nanocrystals [IC-104]
Dmitry Dirin, ETH Zurich
A. Vivani, M. I. Bodnarchuk, M. Aebli, I. Cherniukh, A. Guagliardi, M. V. Kovalenko*

Exploring the chemical scope of light activated protein conjugation using desferrioxamine B derivatives [IC-105]
Daniel F. Earley, University of Zurich
A. Guillou, J. P. Holland*

Reversible Cyclometallation of Aryl-Pya Iridium Complexes [IC-106]
Albert Farre, University of Bern
M. Albrecht*

The introduction of ^{161}Tb to the clinic through the Good Manufacturing Practice compliant production of ^{161}Tb-DOTATOC [IC-107]
Chiara Favaretto, Paul Scherrer Institute (PSI), Villigen
Z. Talip, P. V. Grundler, S. Geistlich, S. Landolt, J. R. Zeevaart, U. Köster, R. Schibli, N. P. van der Meulen*

Development of the matched pair Sc-44/Sc-47 for diagnosis and therapy [IC-108]
Pascal Grundler, Paul Scherrer Institute (PSI), Villigen
R. Hasler, C. Favaretto, Z. Talip, G. Dellepiane, T. S. Carzaniga, S. Braccini, U. Köster, C. Müller, N. P. van der Meulen*

Functionalized single-layer graphene for carbon capture [IC-109]
Kuang-Jung Hsu, EPFL Lausanne

Incorporating vacancy defects in single-layer graphene lattice with a sub-1-Å resolution [IC-110]
Shiqi Huang, EPFL Lausanne
K. V. Agrawal*

DNA-ferrocene as two-step-mechanophore [IC-111]
Emilie Jean-Pierre, University of Fribourg
E. Janett, C. Bochet, K. M. Fromm*

Carbon Dioxide Reductive Disproportionation Driven by Electron-Rich f-Elements Complexes Supported by Heptadentate Non-Innocent Ligands [IC-112]
Nadir Jori, EPFL Lausanne
M. Falcone, D. Toniolo, R. Scopelliti, M. Mazzanti*

Shedding light on Lithium-Alkoxide Mediated Magnesium-Bromine Exchange Reaction [IC-113]
Neil Judge, University of Bern

Scale-up of gas-sieving nanoporous single-layer graphene membrane[1] [IC-114]
Wan-Chi Lee, EPFL Lausanne
K. V. Agrawal

Metal soap membranes for gas separation [IC-115]
Qi Liu, EPFL

Direct Co-H exchange of Fluoroarenes mediated by a mixed-metal Na/Co(II) base [IC-116]
Alessandra Logallo, University of Bern
E. Hevia*

New compounds and superconductors in the η-carbide family [IC-117]
Keyuan Ma, University of Zurich
F. O. von Rohr*

Mixed Alkali-Zinc Bases in Direct Metallation: Alkyl Versus Amide Kinetic Basicity and Stabilization of Delicate Fluoroarene Anions [IC-118]
Pasquale Mastropierro, University of Bern
M. Uzealc, E. Hevia*

Cyclic Tetrapeptides for Chelation of Lead [IC-119]
Tagwa Mohammed, University of Zurich
M. Shoshan*

N-heterocyclic carbene iron piano stool complexes for lactide polymerisation catalysis [IC-120]
Pamela V.S. Nylund, University of Bern
M. Albrecht*

Metalla-assemblies for photodynamic therapy [IC-121]
Chrysanthi Papadimou, University of Neuchâtel
B. Therrien*

Spin-flip luminescence in six-coordinate complexes of nickel(II): attempts and challenges [IC-122]
Christian Reber, Université de Montréal
C. Dab, C. Förster, K. Heinze, C. Reber*

Bis(Pyridylidene Admide) Ligands for Highly Efficient Ruthenium-Catalyzed Olefin Oxidation [IC-123]
Kevin Salzmann, University of Bern
C. Segarra, M. Albrecht*

Bioinspired Metal-Complexes as Chelators of Bacterial Metallo-β-Lactamase Zinc Ions [IC-124]
Justine V.R. Schwarte, University of Fribourg
B. Giese*

Synthesis of crystalline atom-thick poly(triazine imide) nanosheets for energy-efficient molecular separation [IC-125]
Luis Villalobos, EPFL Lausanne
K. V. Agrawal*

Stabilizing Molecular Complexes of Terbium(IV) and Accessing Molecular Complexes of Praseodymium in the +IV Oxidation State [IC-126]
Aurélien R. Willauer, EPFL Lausanne
C. T. Palumbo, R. Scopelliti, F. Fadaei-Tirani, I. Zivkovic, I. Douair, L. Maron, M. Mazzanti*

Polymorphism and Polytypism in the NbS_2 System [IC-127]
Catherine Witteveen, University of Zurich
F. O. von Rohr

Medicinal Chemistry & Chemical Biology [MC] Virtual Poster Session

Secondary structure transitions in dephosphorylated phosvitin studied by circular dichroism spectroscopy [MC-101]
Martin Betschart, Albert-Ludwigs-Universität Freiburg
T. Muszer, M. Sarem, S. Lüdeke*, V. Shastri*

Targeted Therapy for Neurological Disorders: A Novel, Orally Available, and Brain-Penetrant mTOR Inhibitor (PQR626) [MC-102]
Chiara Borsari, University of Basel
E. Keles, M. De Pascale, A. Treyer, R. Sriramaratnam, M. Hamburger, P. Hebeisen, D. Fabbro, P. Hillmann, M. P. Wymann*

NMR Studies of Hierarchical Protein Dynamics [MC-103]
Baptiste Busi, EPFL Lausanne
J. R. Yarava, M. Blackledge, H. Oschkinat, L. Emsley*

One Fingerprint to Rule them All: Drugs, the Metabolome, and Biomolecules [MC-104]
Alice Capecchi, University of Bern
D. Probst, J. L. Reymond*

Targeting HIF-2η in Clear Cell Renal Cell Carcinoma with PROTACs [MC-105]
Carlotta Cecchini, University of Geneva

Linker design for targeting the hGRP receptor by radiolabelled bombesin-based peptides [MC-106]
Martina De Foresta, ETH Zurich
N. Romantini, X. Deupi, M. Béhé, H. Wennemers*

Preclinical Development of PQR514, a Highly Potent PI3K Inhibitor Bearing a Difluoromethyl-Pyrimidine Moiety [MC-107]
Martina De Pascale, University of Basel
C. Borsari, D. Rageot, F. Beaufils, T. Bohnacker, E. Keles, A. Melone, P. Hebeisen, D. Fabbro, M. P. Wymann*

High content screening on patient-derived cells to break drug resistance in melanoma targeted therapy [MC-108]
Lara Dürr, University of Basel
T. Hell, M. Dobrzynski, S. Radetzki, A. Mattei, J. P. von Kries, M. Hamburger, O. Pertz, E. Garo

Lipoprotein-mimickry through supramolecular protein engineering [MC-109]
Thomas Edwardson, ETH Zurich
S. Tetter, D. Hilvert*

Peptide Dendrimers Mimicking Glatiramer Acetate [MC-110]
Dina Erzina, University of Bern
A. Capecchi, S. Javor, J. L. Reymond*

Immunological Epitope Mapping of the SARS-CoV-2 Spike Protein [MC-111]
Lluc Farrera Soler, University of Geneva
S. Barluenga, J. Daguer, N. Winssinger*

Increasing fluorophore brightness through self-labeling protein tags [MC-112]
Michelle Frei, EPFL Lausanne
M. Tarnawski, J. Hiblot, K. Johnsson*

New anti-inflammatory and pro-apoptotic photosensitizers against arthritis [MC-113]
Manuel Gallardo-Villagran, University of Neuchâtel
D. Léger, B. Therrien*, B. Liagre*

Fluorescent Probes for Measuring Membrane Tension, towards Super-Resolution Microscopy [MC-114]
José García-Calvo, University of Geneva
J. Maillard, I. Fureraj, K. Strakova, A. Colom, V. Mercier, A. Roux, E. Vauthey, N. Sakai, A. Fürstenberg*, S. Matile*

Functionalization of harmonic nanoparticles for ultra-sensitive imaging and theranostic applications [MC-115]
Adrian Gheata, EPFL Lausanne
R. de Matos, J. Vuilleumier, L. Bonacina, S. Gerber-Lemaire*

Novel Monovalent Ligands for Siglec-8, a Promising Target for Eosinophil and Mast Cell Related Disorders [MC-116]
Benedetta Girardi, University of Basel
G. Conti, J. Cramer, B. Kroezen, S. Rabbani, T. Tomasic, M. Anderluh, J. Mravljak, D. Ricklin, O. Schwardt*, B. Ernst*

AI-based design and synthesis of putative HtrA inhibitors [MC-117]
Alissa Götzinger, ETH Zurich
D. Montero Salas, M. Orsi, A. L. Button, F. Grisoni, G. Schneider*

Peptide Stapling via Selective Cysteine Alkynylation Using Hypervalent Iodine Reagents [MC-118]
Elija Grinhagena, EPFL Lausanne
J. Ceballos, J. Waser*

Bioorthogonal site-selective conjugation of fluorescent dyes to antibodies: method and potential applications [MC-119]
Philipp Grossenbacher, University of Bern
S. A. Singer, J. Moser, S. A. Bernhard, B. Stieger, M. Lochner*

Optimization of Antimicrobial Peptide Dendrimers Using a Genetic Algorithm [MC-120]
Xingguang Cai, University of Bern
A. Capecchi, S. Javor, J. L. Reymond*

Synthesis and Reactivity of Colibactin Inspired 1,6-Michael Acceptor [MC-121]
Agron Ilazi, University of Zurich
K. Gademann*

^{1}H HR-MAS NMR Based Metabolic Profiling of Cells in Response to Treatment with the Photosensitizer Chlorin e4 with and without Polymeric Carrier Systems [MC-122]
Tobias Kämpfer, University of Bern
P. Vermathen*, M. Vermathen*

Model Peptide Studies of Ag^{+} Binding Sites Inspired by the Silver Resistance Protein SilE [MC-123]
Florian Marquenet, University of Fribourg
L. Babel, V. Chabert, K. M. Fromm*

Synthesis and biological evaluation of PROTACs and destabilizers with putative anti-inflammatory activity [MC-124]
Sara Pannilunghi, University of Geneva

Bio-inspired divergent synthesis of various sesquiterpene including Goyazensolide, its new cellular target and its therapeutic potential in cancer and virology [MC-125]
Remi Patouret, University of Geneva
W. Liu, S. Barluenga, M. Planck, R. Loewith*, N. Winssinger*

X-Ray Crystallographic Studies of Short Antimicrobial Helical Peptides against Multidrug Resistant Gram-Negative Bacteria [MC-126]
Hippolyte Personne, University of Bern
S. Baeriswyl, A. Stocker, S. Javor, J. L. Reymond*

Solving the X-ray structure of a bio-artificial neurotransmitter receptor designed for the naked-eye recognition of dopamine [MC-127]
Thibaud Rossel, Gymnase français de Bienne
R. Gobat, B. Zhang

The effects of chemical reactions on codon drift in DNA encoded libraries [MC-128]
Basilius Sauter, University of Basel
L. Schneider, C. Stress, D. Gillingham*

Antibiotic Delivery via Disulfide Exchange [MC-129]
Inga Shchelik, University of Zurich
K. Gademann*

Exploring the role of CEMIP in Alport syndrome [MC-130]
Sofia Spataro, University of Geneva
J. Sgrignani, A. Cavalli, L. Scapozza, M. Prunotto

Structural investigation of the first unimolecular RNA G-quadruplex via NMR spectroscopy [MC-131]
Zenghui Wang, University of Zurich
S. Johannsen, A. Dominguez-Martin, R. K. Sigel*

Peptide dendrimers for cisplatin delivery to cancer cells [MC-132]
Elena Zakharova, University of Bern
S. Javor, J. L. Reymond*

Peptide-based vectors for delivery of pDNA encoding CRISPR/Cas9 in 3D tumor spheroids [MC-133]
Susanna Zamolo, University of Bern
T. Darbre*, J. L. Reymond*

Organic Chemistry [OC] Virtual Poster Session

Anti-Markovnikov Oxyalkynylation of Ene-carbamates and Enol-ethers under Photoredox Catalysis [OC-101]
Stephanie Amos, EPFL Lausanne
S. Nicolai, J. Waser*

A Rhodium(III)-Catalyzed Cyclopropane C-H/C-C Activation Sequence Provides Diastereoselective Access to α-Alkoxylated γ-Lactams [OC-102]
Benoit Audic, EPFL Lausanne
N. Cramer*

One-Pot Alkene Hydroboration – Palladium Catalyzed Migratory Suzuki – Miyaura C(sp^3) – C(sp^2) Cross-Coupling [OC-103]
Yann Baumgartner, University of Basel
O. Baudoin*

Ficini-Type Reactions with 1-Alkynyltriazenes [OC-104]
Carl Bormann, EPFL Lausanne
K. Severin*

Synthesis of Functionalized β- and γ-Hydroxy Sulfides by Oxy-Alkynylation of Thiiranes and Thietanes [OC-105]
Julien Borrel, EPFL Lausanne
G. Pisella, J. Waser*

A Chiral Naphthyridine Diimine Ligand Platform Enables Nickel-Catalyzed Asymmetric Alkylidenecyclopropanations [OC-106]
Elena Braconi, EPFL Lausanne
N. Cramer*

Organocatalyzed Conjugate Addition Reactions of Aldehydes to Nitroolefins with *Anti*-Selectivity [OC-107]
Alena Budinská, ETH Zurich
T. Schnitzer, H. Wennemers*

Synthesis of Amides and Esters *via* Pd^0-Catalyzed Carbonylative C(sp^3)-H Activation / 1,4-Pd Shift [OC-108]
Tomáš Čarný, University of Basel
R. Rocaboy, A. Clemenceau, O. Baudoin*

Direct Synthesis of Cyclopropanes from gem-Dialkyl Groups through Double C–H Activation [OC-109]
Antonin Clemenceau, University of Basel
P. Thesmar, O. Baudoin*

Palladium-Catalyzed Di-functionalization of Allylic Amines and Alcohols Using Aldehyde-Derived Tethers [OC-110]
Ashis K. Das, EPFL Lausanne
S. Nicolai, J. Waser*

Hypervalent Iodine Reagents as Oxy-Allyl Cation Synthetic Equivalents for the Synthesis of Vinyl Ethers and Ketones [OC-111]
Nina Declas, EPFL Lausanne
J. Waser*

Studying the Effectiveness of Lithium Zincates Species in Michael Addition Reactions: Synthetic and Structural Insights [OC-112]
Marzia Dell'Aera, University of Bern
A. Altomare, V. Capriati*, E. Hevia*

Bicyclopyrone-Synthesis of a Modern Herbicide [OC-113]
Andrew J. F. Edmunds, Syngenta Crop Protection AG
R. G. Hall, W. T. Rueegg, A. De Mesmaeker , R. H. Beaudegnies

Functionalizable peptide-coated PtNPs for targeting liver cancer cells [OC-114]
Elisabeth Engelsberger, ETH Zurich
M. Shoshan, H. Wennemers*

Through Bond and Space: Curved Light Harvesting Arrays [OC-115]
Lucia Gallego, University of Zurich
M. Rickhaus*

Transition-Metal-Free Arylation of *N,O*-Acetals Using Cooperative Zn/Zn Partnerships [OC-116]
Jose Gil-Negrete, University of Bern
E. Hevia*

Pnictogen-Bonding Catalysis: Polyether Cyclizations
Andrea Gini, University of Geneva
M. Paraja, B. Galmés, C. Besnard, A. I. Poblador-Bahamonde, N. Sakai, A. Frontera, S. Matile*

PhotoTags: Photoactivatable fluorophores for protein labelling [OC-118]
Amaury Guillou, University of Zurich
J. P. Holland*

Stereoselective Synthesis of Atropoisomeric Biaryls [OC-119]
Zlatko Jončev, University of Basel
C. Sparr*

Switching of Chromophores in Optical Antennas [OC-120]
Laurent Jucker, University of Basel
M. Ochs, R. Kullock, M. Mayor*, B. Hecht*

New Neo-Clerodane Diterpenes from *Teucrium polium* [OC-121]
Morris Keller, University of Basel
S. Chabane, A. Boudjelal, M. Hamburger, O. Potterat*

Synthesis of a Macrocyclic Gold Atom Acceptor [OC-122]
Charlotte Kress, University of Basel
P. Zwick, M. Mayor*

Brønsted and Lewis acid adducts of triazenes [OC-123]
Iris Landman, EPFL Lausanne
A. A. Suleymanov, K. Severin*

C-Terminal Oxidative Decarboxylative Functionalization of Peptides: a Toolbox Towards Structural Diversity [OC-124]
Eliott Le Du, EPFL Lausanne
M. Garreau, J. Waser*

Iron-catalysed Remote C(sp^3)-H Azidation of *O*-acyl Oximes and *N*-acyloxy Imidates [OC-125]
Alexandre Leclair, EPFL Lausanne
R. O. Torres-Ochoa, Q. Nguyen, J. Zhu*

[2^n]Cyclophane carbon nanohoops [OC-126]
Juraj Malinčík, University of Basel
K. Reznikova, T. Šolomek*

A Conformationally Tailored Peptide Catalyst Allows for Amine Catalysis with N-Heterocyclic Moieties [OC-127]
Jasper S. Möhler, ETH Zurich
T. Schnitzer, H. Wennemers*

At the Core of Dynamic Polymers: The Self-Assembly of Twisted Aryl Amines [OC-128]
Melissa Nehme, University of Zurich
M. Rickhaus*

Intermolecular Palladium(0)-Catalyzed Atropo-enantioselective C-H Arylation of Hereroarenes [OC-129]
Qui-Hien Nguyen, EPFL Lausanne

Synthesis and Characterization of new chiral Bifunctional NHC-Complexes [OC-130]
Nadja Niggli, University of Basel
O. Baudoin*

Primary Anion-π Catalysis of Epoxide-Opening Ether Cyclizations: Access to New Reactivity and Natural Product Inspired Cascades [OC-131]
Miguel Paraja, University of Geneva
X. Hao, S. Matile*

Cethrenes – Chiroptical & magnetic switches for supramolecular conductive assemblies [OC-132]
Tomáš Pastierik, University of Zurich
P. Ribar, C. Schuppisser, M. Juríček*

Annulation of D-A Aminocyclopropanes: Efficient Activation without the Need for a Diester Group [OC-133]
Vincent Pirenne, EPFL Lausanne
J. Waser*

Three-Component Oxy-Alkynylation of Diazo Compounds: Synthesis of Highly Functionalized Propargyl Ethers[1] [OC-134]
Guillaume Pisella, EPFL Lausanne
A. Gagnebin, J. Waser*

Molecular tethering for Pd catalyzed stereoselective difunctionalization of unsaturated systems [OC-135]
Mikus Purins, EPFL Lausanne
L. Buzzetti, P. Greenwood, J. Waser*

Synthesis and biological profile of all stereoisomers of GR24-lactam and analogues [OC-136]
Pierre Quinodoz, Syngenta Crop Protection AG
A. Lumbroso, M. Lachia, C. Screpanti, S. Rendine, S. Catak, R. Fonné-Pfister, K. Hermann, A. De Mesmaeker *

Tailor-Made Molecular Rods for Graphene Junctions [OC-137]
Ksenia Reznikova, University of Basel
L. Delarue Bizzini, M. El Abbassi, O. Schmuck, A. Christy, D. Häussinger, M. Neuburger, M. Calame, M. Mayor*

Enantioselective C(sp^2)-H arylation for the synthesis of warped molecules [OC-138]
Davd Savary, University of Basel
O. Baudoin*

Emergence of Complex Molecular Systems *via* Combination of Covalent and Non-Covalent Synthesis [OC-139]
Tobias Schnitzer, Eindhoven University of Technology
E. W. Meijer*

Peptide catalyzed stereoselective conjugate addition reaction of aldehydes to fluorinated nitroolefins [OC-140]
Martin Schnurr, ETH Zurich
H. Wennemers*

Green, π-Acidic Naphthalenediimides with Oligosulfides in Their Core [OC-141]
Inga Shybeka, University of Geneva
A. Aster, N. Sakai, A. Frontera, E. Vauthey, S. Matile*

Towards Molecular Graphene Belts and Möbius Strips [OC-142]
Eric Sidler, University of Basel
M. Mayor*

A highly sensitive and selective colorimetric and fluorescent sensor for phosgene detection [OC-143]
Atena Solea, University of Fribourg
A. Crochet, C. Allemann, K. M. Fromm, O. Mamula*

Highly Divergent Access to Densely Substituted Arenes, Pyridines and Pyridones *via* Transition Metal-Catalyzed Transformations of Alkynyl Triazenes [OC-144]
Jin Tan, EPFL Lausanne
C. T. Bormann, F. Perrin, M. F. Chadwick, K. Severin*, N. Cramer*

Synthesis and Characterisation of Metallo-Porphyrin Dyads [OC-145]
Jan Thiede, University of Bern
R. Ingle, M. Chergui, S. Liu, R. Häner*

Continuous flow chemistry methodologies to support UCB drug discovery [OC-146]
Matthieu Tissot, UCB biopharma

Remote C(sp^3)-H Functionalization Enabled by Transition Metals [OC-147]
Rubén O. Torres-Ochoa, Universidad Nacional Autónoma de México
A. Leclair, Z. Li, Q. Wang, J. Zhu*

Assessment of the Synthetic Feasibility of Generated Chemical Space by Computer Assisted Synthesis Planning [OC-148]
Amol Thakkar, University of Bern
V. Chadimova, E. J. Bjerrum, O. Engkvist, J. L. Reymond*

Catalytically Active Peptides For Conjugate Addition Reactions with *C*-substituted Maleimides [OC-149]
Greta Vastakaite, ETH Zurich
H. Wennemers*

Thermal and Electrical Transport Through Organic Radicals: Taking Advantage of the Kondo Effect [OC-150]
David Vogel, University of Basel
C. Hsu, M. Mayor*, H. van der Zant *

Oxidative ring-opening fluorination of cyclopropylamides [OC-151]
Ming-Ming Wang, EPFL Lausanne
J. Waser*

Cethrenes: Self-assembly of magnetic conducting molecular wires [OC-152]
Yujia Wang, University of Zurich
M. Juríček*

Synthesis of Carpyridines [OC-153]
Joseph Woods, University of Zurich
M. Rickhaus*

Access to *P*- and Axially Chiral Biaryl Phosphine Oxides by Enantioselective Cp^xIr^{III}-Catalyzed C-H Arylations [OC-154]
Łukasz Woźniak, EPFL Lausanne
Y. S. Jang, J. Pedroni, N. Cramer*

Pd^0-catalyzed Enantioselective Intramolecular Arylation of Enantiotopic Secondary C–H Bonds [OC-155]
Marco Zuccarello, University of Basel
R. Melot, D. Cavalli, N. E. Niggli, O. Baudoin*

Physical Chemistry [PC] Virtual Poster Session

Synthesis and luminescence peoperties of strontium aluminate nanospheres as long persistent phosphors [PC-101]
Jafar Afshani, University of Geneva
T. Delgado

Dynamic Nuclear Polarisation Enhancement of 200 at 21.15 T Enabled by 65 kHz Magic Angle Spinning [PC-102]
Pierrick Berruyer, EPFL Lausanne
S. Björgvinsdóttir, A. Bertarello, G. Stevanato, Y. Rao, O. Ouari, M. Lelli, F. Engelke, L. Emsley*

Surface and bulk hyperpolarization of lithium titanates [PC-103]
Snaedis Björgvinsdóttir, EPFL Lausanne
P. Moutzouri, P. Berruyer, M. A. Hope, L. Emsley*

Insight into the crystallization of $MgCO_3$ grown by CO_2 capture on (100)-MgO promoted by $NaNO_3$ [PC-104]
Alexander Bork, ETH Zurich
M. Rekhtina, E. Willinger, C. R. Müller*, P. M. Abdala*

Data mining chemical shifts in the solid state for automated assignment of organic crystals [PC-106]
Manuel Cordova, EPFL Lausanne
M. Balodis, B. Simões de Almeida, L. Emsley*

Analytic calculation and analysis of Atomic Polar Tensors for Molecules and Materials [PC-107]
Edward Ditler, University of Zurich
S. Luber*

Temperature dependence of intermolecular correlations in bulk water and electrolyte solutions [PC-108]
Nathan Dupertuis, EPFL Lausanne
Y. Chen, H. I. Okur, S. Roke*

Dispersion effects described by the Frozen-Density embedding Theory [PC-109]
Mingxue Fu, University of Geneva
C. E. Gonzalez, N. Ricardi, T. A. Wesolowski

Femtosecond broadband fluorescence upconversion spectroscopy to study vibrational energy relaxation dynamics in organic molecules in solution [PC-110]
Ina Fureraj, University of Geneva
E. Vauthey*

Cryogenic Ion Vibrational Predissociation (CIVP) Spectroscopy of a Gas-phase Molecular Torsion Balance to probe London dispersion Forces in Large Molecules [PC-111]
Vladimir Gorbachev, ETH Zurich
A. Tsybizova, L. Fritsche, L. Miloglyadova, P. Chen*

NMR Crystallography Determines the Supramolecular Structure of Layered Hybrid Perovskites [PC-112]
Michael Hope, EPFL Lausanne
A. Mishra, M. Cordova, J. V. Milic, T. Nakamura, P. Ahlawat, D. J. Kubicki, C. E. Avalos, U. Roethlisberger, M. Graetzel*, L. Emsley*

Residual Gas Effects on the Gas Chromatographic Yield of Mercury and Astatine, and Their Impact on the Study of Transactinides Copernicium and Flerovium [PC-113]
Paul Ionescu, University of Bern
N. V. Aksenov, G. A. Bozhikov, N. M. Chiera, R. Dressler, S. N. Dimitriev, P. Steinegger, A. Türler*, R. Eichler*

High Resolution Infrared Spectroscopy of Cyano-oxirane (c-C_2H_3OCN) [PC-114]
Karen Keppler, ETH Zurich
S. Albert, Z. Chen, P. Lerch, C. Manca Tanner, J. Stohner, M. Quack*

Dynamic second-harmonic imaging of lipid membrane hydration [PC-115]
Seonwoo Lee, EPFL Lausanne
D. Roesel, M. Eremchev, S. Roke*

Surface segregation and selective oxidation of CuIn near surface alloys under CO_2 hydrogenation conditions: a near ambient pressure XPS study [PC-116]
Mo Li, EPFL Lausanne
A. Züttel, W. Luo*

Insights on the formation of nanopores in single-layer graphene [PC-117]
Shaoxian Li, EPFL Lausanne
S. Huang, M. Rezaei, K. V. Agrawal*

Super-Resolution Microscopy with Mechanosensitive Membrane Tension Probes [PC-118]
Jimmy Maillard, University of Geneva
J. García-Calvo, K. Strakova, N. Sakai, S. Matile, A. Fürstenberg*

Hybrid Trapping of Stark-Decelerated Polar Molecules and Laser-Cooled Ions in a Cryogenic Trap [PC-119]
Christian Mangeng, University of Basel
T. Kierspel, C. von Planta, D. Haas, D. Zhang, S. Willitsch*

Intermediate Phase During Perovskite Crystallization Revealed using solid-state NMR [PC-120]
Aditya Mishra, EPFL Lausanne
D. J. Kubicki, C. E. Avalos, J. Zhang, Z. Wang, A. Hagfeldt, M. Graetzel*, L. Emsley*

Why is this chiral Europium complex such a good CPL emitter? New insights from time-resolved CD spectroscopy [PC-121]
Livia Müller, EPFL Lausanne
B. Bauer, F. Zinna, M. Chergui, M. Oppermann*

Investigating State-Specific and Conformational Effects in Penning Ionisation Reactions [PC-122]
Ludger Ploenes, University of Basel
P. Stranak, H. Gao, J. Küpper, S. Willitsch*

Exciton and multi-excitons recombination dynamics in perovskite $CsPbBr_3$ QDs unveiled by single QD optical spectroscopy [PC-123]
Gabriele Raino, ETH Zurich
F. Krieg, M. I. Bodnarchuk, M. V. Kovalenko*

***In situ* pair distribution function analysis of the decomposition pathways of hydrated magnesium hydroxycarbonate in the presence of sodium nitrate [PC-124]**
Margarita Rekhtina, ETH Zurich
D. Stoian, A. Fedorov, P. M. Abdala*, C. R. Müller*

Label-free and charge-sensitive second-harmonic imaging of giant vesicle hydration [PC-125]
David Roesel, EPFL Lausanne
M. Eremchev, S. Roke*

Using Ultrafast Spectroscopy and Computer Simulations to Re-examine Our Picture of Photoinduced Electron Transfer [PC-126]
Christopher Rumble, University of Geneva
E. Vauthey*

Lipid membrane phase transitions involve structural redistribution of interfacial water [PC-127]
Tereza Schonfeldova, EPFL Lausanne
H. I. Okur, F. Kovacik, S. Roke*

Self-assembled peptide-based nanoparticles for the delivery of nucleic acids [PC-128]
Tarvirdipour Shabnam, University of Basel
C. G. Palivan*

Quantum-non-demolition state detection and spectroscopy of single trapped molecules [PC-129]
Aleksandr Shlykov, University of Basel
M. F. Roguski, M. Sinhal, Z. Meir, S. Willitsch*

3rd order Average Hamiltonian Theory analytical expression for 2 and 3 spins systems in solid-state NMR [PC-130]
Bruno Simões de Almeida, EPFL Lausanne
P. Moutzouri, G. Stevanato, L. Emsley*

Probing liquid interfaces with room-temperature ionic liquids using the excited-state dynamics of a cationic dye [PC-131]
Jihad Sissaoui, University of Geneva
D. Budkina, E. Vauthey*

Towards high precision half-life measurements of exotic radio-lanthanides [PC-132]
Nadine Chiera, Paul Scherrer Institute (PSI), Villigen
R. Dressler, Z. Talip, P. Sprung, A. Fankhauser, D. Schumann*

Excited-state symmetry breaking in multibranched donor-acceptor dyes – The effect of quadrupole moment [PC-133]
Zoltán Szakács, University of Geneva
E. Vauthey*

Infrared Spectroscopy of Chemisorbed Methylidyne coadsorbed with Hydrogen on Pt(211) [PC-134]
Harmina Vejayan, EPFL Lausanne
A. Gutiérrez-González, R. D. Beck*

Proton Transfer in a Propyl Acetate/Butyronitrile Mixture [PC-135]
Pragya Verma, University of Geneva
T. Kumpulainen*

Conformationally and state-controlled ion-molecule reactions [PC-136]
Lei Xu, University of Basel
A. Kilaj, S. Willitsch*

A Formulation Protocol with Pyridine to Enable DNP-SENS on Reactive Surface Sites: Case Study with Olefin Polymerization and Metathesis Catalysts [PC-137]
Alexander Yakimov, ETH Zurich
D. Mance, K. Searles, C. Copéret*

Transfer of Nanoscale Objects into Giant Plasma Membrane Vesicles (GPMVs) serving as cellular model systems [PC-138]
Luisa Zartner, University of Basel
M. Garni, I. Craciun, T. Einfalt, C. G. Palivan*

A donor-acceptor ensemble: merging of TTF and dipyrrolylquinoxaline difluoroborate chemistry [PC-139]
Ping Zhang, University of Bern
U. Aschauer, T. Feurer , R. Häner, S. Liu

Polymers, Colloids & Interfaces [PI] Virtual Poster Session

Conjugated Polymers via Cyclopentannulation Reaction: Promising Materials for Iodine Adsorption [PI-101]
Noorullah Baig, Gulf University for Science and Technology
S. Shetty, S. Al-Mousawi, B. Alameddine*

Conjugated Copolymers Bearing 2,7-Dithienylphenanthrene-9,10-dialkoxy Units: Highly Soluble and Stable Deep-Blue Emissive Materials [PI-102]
Noorullah Baig, Gulf University for Science and Technology
S. Shetty, S. Fall, T. Heiser, B. Alameddine*

Tuning Solid-State Emission from a Single Fluorophore by Controlled Radical Polymerization [PI-103]
Yinyin Bao, ETH Zurich
Y. Bao*

Energy Transfer in DNA-Organized, Multi-Segmental Chromophore Stacks [PI-104]
Nutcha Bürki, University of Bern
E. Grossenbacher, C. D. Bösch, M. Nazari, A. Cannizzo, T. Feurer, S. M. Langenegger, R. Häner*

Efficient Synthesis and Complex Self-Assembly of the Amphiphilic PEO-*b*-PEHOx polymers into Multicompartment Micelles, Pseudo-Vesicles and Yolk/Shell Nanoparticles [PI-105]
Davy Daubian, University of Basel
J. Gaitzsch, W. Meier*

Spatiotemporal imaging of water in operating voltage-gated ion channels reveals the slow motion of interfacial ions [PI-106]
Maksim Eremchev, EPFL Lausanne
O. Tarun, A. Radenovic, S. Roke*

Light-Harvesting Antenna: Detection of Polyaromatic Molecules by Supramolecular Fibers [PI-107]
Jovana Jevric, University of Bern
S. M. Langenegger, R. Häner*

Phase-Separated Metallosupramolecular Polymer Blends with Tunable Mechanical Properties [PI-108]
Franziska Marx, University of Fribourg, Adolphe Merkle Institute
J. Sautaux, L. Neumann, C. Weder*, S. Schrettl*

Functional insertion and characterization of hexameric resorcinarene capsules into solid-supported, synthetic membranes for use as biomimicking surface and ion carrier [PI-109]
Moritz Muthwill, University of Basel
S. Yorulmaz Avsar, S. F. Merget, K. Tiefenbacher*, C. G. Palivan*

Polyphenylene Networks Containing Triptycene Units: Promising Porous Materials for CO_2, CH_4, and H_2 Adsorption [PI-110]
Suchetha Shetty, Gulf University for Science and Technology
N. Baig, A. Hassan, S. Al-Mousawi, N. Das, B. Alameddine*

PBO-*b*-PG Self-assemblies: a Straightforward Path towards Biomedically Relevant Nanoparticles [PI-111]
Riccardo Wehr, University of Basel
J. Gaitzsch, D. Daubian, C. Fodor, W. Meier*

Mechanoresponsive Ag@SiO_2 nanorattles-polymer antimicrobial nanocomposites [PI-112]
Philippe Yep, University of Fribourg
S. L. Abram, K. M. Fromm*

Molecular capsule catalysis: Ready to address current challenges in synthetic organic chemistry? [PS-001]
Konrad Tiefenbacher, University of Basel
L. D. Syntrivanis, I. Némethová, R. T. Li

Development of the Commercial Manufacturing Process for Ipatasertib [PS-002]
Andreas Schuster, F. Hoffmann-La Roche Ltd.
S. Bachmann, H. Iding, C. Lautz, I. Thomé-Pfeiffer, C. Maierhofer, R. Mondière, P. Schmidt, C. Strasser

Tailored Catalysis for the F&F Industry [PS-003]
Denis Jacoby, Firmenich SA

Natural Product Sciences in Modern Drug Discovery and Paths to the Future [PS-004]
Frank Petersen, Novartis Pharma AG

Discovery of a new medicine Risdiplam, a Survival of Motor Neuron-2 *(SMN2)* gene splicing modifier for the treatment of Spinal Muscular Atrophy (SMA) [PS-005]
Hasane Ratni, F. Hoffmann-La Roche Ltd.

Discovery and Optimization of Enantioselective Catalysts through Chemoinformatics [PS-006]
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The complete program and all abstracts are available as interactive application on *http://scg.ch/fallmeeting/2020*