

University of Zurich  
Irchel Campus  
Winterthurerstrasse 190  
CH-8057 Zürich



Thu, 15 September 2016, 09.00 – 18.30

# SCS Fall Meeting 2016

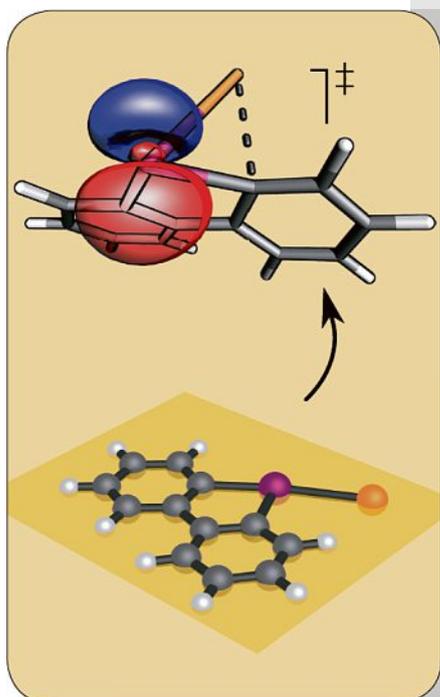
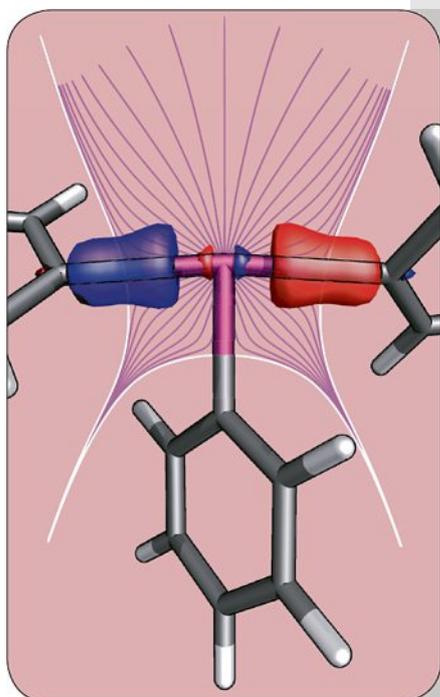
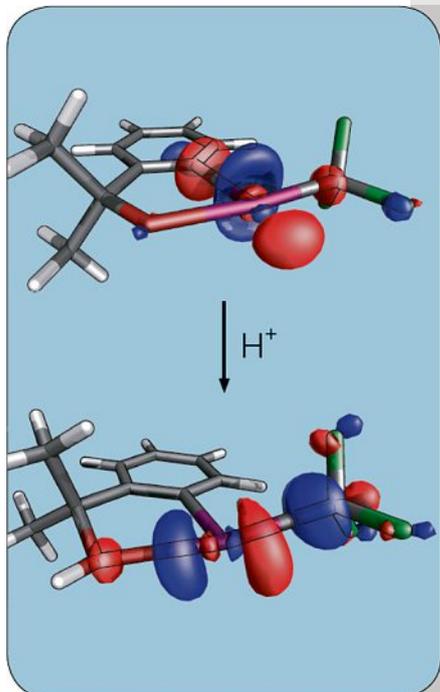
- 09.00 Welcome Coffee  
Registration and poster installation
- 09.45 Welcome and conference opening
- 09.55 Invited Lecture by *Prof. E Peter Kündig*  
SCS Honorary Member 2016
- 10.30 Sandmeyer Award Lecture 2016  
*Dr. Martin Weibel, Dr. Robert Flatt, Dr. Hendrik Heinz,*  
Sika Technology AG
- 11.00 Break
- 11.15 Morning Parallel Session
- Analytical Sciences (AS)
  - Catalysis Science & Engineering (CE)
  - Computational Chemistry (CC)
  - Inorganic & Coordination Chemistry (IC)
  - Medicinal Chemistry & Chemical Biology (MC)
  - Organic Chemistry (OC)
  - Physical Chemistry (PC)
  - Polymers, Colloids & Interfaces (PI)
- 12.45 Lunch and Poster Session  
Commercial Exhibition
- 15.00 Afternoon Parallel Session  
Same structure and locations as morning session  
Exhibitor Aperitif
- 16.45 Break and coffee/refreshments
- 17.00 Paracelsus Award Lecture 2016  
*Prof. Michael Graetzel,* EPF Lausanne,
- 18.00 Best Presentation Award Ceremonies
- 18.30 End of the conference

<http://scg.ch/fallmeeting/2016/>

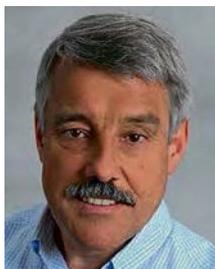


Universität  
Zürich<sup>UZH</sup>

**ETH** zürich



## WELCOME TO THE 2016 FALL MEETING OF THE SWISS CHEMICAL SOCIETY (SCS)



Hans Peter Lüthi

On behalf of the Division of Chemical Research of the Swiss Chemical Society, we welcome you to the 2016 Fall Meeting, hosted jointly by the ETH Zurich and the University of Zurich Departments of Chemistry at the Irchel Campus. We also welcome the presenters of the nearly six-hundred scientific contributions (posters, contributed lectures, invited lectures), many of them graduate students and post-doctoral fellows.

We will also have a number of invited lectures presented by distinguished scientists. This year's Fall Meeting will open with the lecture of Peter Kündig, former president and now honorary member of the SCS, followed by the Sandmeyer Award Lecture presented by Robert Flatt and his team of Sika. Other invited and award lectures, including the SCS-KGF Award Lectures, will be delivered in the Parallel Sessions.

One of the highlights of the Fall Meeting will be the Paracelsus Award Lecture presented by Michael Graetzel of EPFL, followed by the Award Ceremony for the best oral and poster contributions, where more than twenty prizes will be handed out to their winners.

At the Commercial Exhibition, twenty companies will be presenting their products and services. At the same time, there will also be the Poster Session.

This year, we particularly welcome the participants of the first symposium 'Future of Chemical Education' for instructors of chemistry at all levels. Being part of the Fall Meeting, the symposium is expected to help build bridges between research and education. As a young participant watch out: your former high school teacher may be part of your audience!

We are grateful to our sponsors for their continued support. This support is also an expression of the interest of industry in our research activities, many of which are carried out by young scientists.

We invite you to browse through the program and hope that the 2016 Fall Meeting will capture your interest. Your participation and your contribution to the scientific discussion will help to make the event a success for everybody involved.

We look forward to seeing you on Thursday, September 15 at the University of Zürich Irchel Campus!



Christian Bochet

Prof. Christian Bochet  
Chairman of the Division of  
Chemical Research

PD Dr. Hans Peter Lüthi  
Chairman of the Organizing Committee

## DEAR PARTICIPANTS OF THE FALL MEETING OF THE SWISS CHEMICAL SOCIETY



Michael Hengartner

Chemistry has a long and successful tradition in Zurich: The University of Zurich was home to several renowned chemists, including Alfred Werner and Paul Karrer, who were awarded the Nobel Prize in Chemistry in 1913 and 1937, respectively. Today, the Department of Chemistry is known for its broad, interdisciplinary research that guarantees an optimal education in chemistry and fields related to chemistry.

As President of UZH, I am therefore all the more pleased that the Swiss Chemical Society regularly holds its annual Fall Meeting at our institution and that young chemists, graduate students, and postdoctoral fellows from throughout Switzerland come to UZH to discuss and present their latest research. For this year's conference, an impressive number of almost 600 scholarly contributions have been submitted.

As in previous years, the 2016 Zurich Fall Meeting is organized by a team of scientists from the University of Zurich and ETH Zurich – a perfect example of how collaboration brings benefits to scholarship. UZH is proud to host this conference on our University's Irchel Campus; with its beautiful outdoor environment and bright, modern buildings, the campus provides an excellent venue for the meeting.

I extend a warm welcome to the University of Zurich and wish you a stimulating and successful conference. There are certain to be many outstanding contributions and interesting discussions – all in an atmosphere that inspires both scholarly collaboration and personal friendship.

Prof. Michael Hengartner  
President of the University of Zurich

## THE SCS FALL MEETING – A SUCCESS STORY



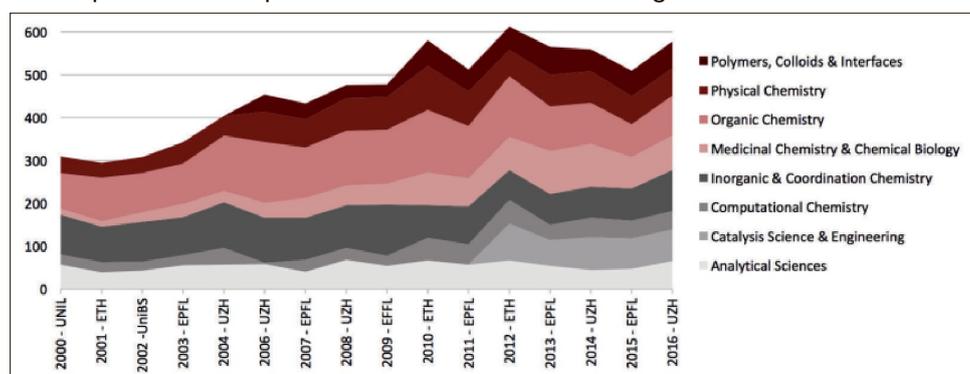
David Spichiger

On an annual basis, right before the start of the new academic year, the Swiss Chemical Society holds its traditional Fall Meeting. It has developed into one of the biggest and most renowned annual, scientific meetings in Switzerland and provides a platform for junior and senior researchers, for academics and industrials, and for scientists of almost all fields of chemistry.

In the late 19<sup>th</sup> century the chemical community was part of the 'Schweizerische Naturforschende Gesellschaft (SNG)' and the chemists met to form one of the five SNG sections (botany, zoology, geology, physics/mathematics, chemistry). The increasing importance of chemistry motivated Profs. Werner, Bamberger and Billeter to create their own society and after the foundation of the Swiss Chemical Society in 1901, the General Assemblies of the Society took place after the summer vacations. As the members were not very interested in the society's business, the president and his board colleagues decided to increase the assembly's attractiveness by including some scientific talks before and after the statutory parts. This marks the beginning of today's SCS Fall Meetings.<sup>[1]</sup>

Since 2000, the number of abstracts has increased from about 300 to almost 600. We have also successfully implemented two new sessions: Polymers, Colloids & Interfaces and Catalysis & Engineering. Most recently, we launched a new initiative which aims at the implementation of a chemical education session (seminar/workshops). Its first edition is part of the SCS Fall Meeting 2016.

Development of accepted abstracts at the Fall Meeting from 2000 to 2016



Abstracts at the Fall Meeting 2016 per Session

	Posters	Talks/ Lectures	Total Contributions	0	20	40	60	80	100
Analytical Sciences	54	11	65	[Bar chart showing 65 total contributions]					
Catalysis Science and Engineering	62	11	73	[Bar chart showing 73 total contributions]					
Computational Chemistry	33	11	44	[Bar chart showing 44 total contributions]					
Inorganic Chemistry	84	11	95	[Bar chart showing 95 total contributions]					
Medicinal Chemistry & Chemical Biology	68	13	81	[Bar chart showing 81 total contributions]					
Organic Chemistry	82	11	93	[Bar chart showing 93 total contributions]					
Physical Chemistry	53	12	65	[Bar chart showing 65 total contributions]					
Polymers, Colloids and Interfaces	51	11	62	[Bar chart showing 62 total contributions]					
Plenary Session	0	4	4	[Bar chart showing 4 total contributions]					
<b>Grand Total</b>	<b>487</b>	<b>94</b>	<b>582</b>						

Abstracts at the Fall Meeting 2016 per Affiliation

	Posters	Talks/ Lectures	Total Contributions	0	20	40	60	80	100	120	140	160
ETH Zurich	128	19	147	[Bar chart showing 147 total contributions]								
EPF Lausanne	66	8	75	[Bar chart showing 75 total contributions]								
University of Basel	57	11	68	[Bar chart showing 68 total contributions]								
University of Bern	41	3	44	[Bar chart showing 44 total contributions]								
University of Fribourg	25	5	30	[Bar chart showing 30 total contributions]								
University of Geneva	40	6	47	[Bar chart showing 47 total contributions]								
University of Neuchatel	4	0	4	[Bar chart showing 4 total contributions]								
University of Zurich	49	8	57	[Bar chart showing 57 total contributions]								
Paul Scherrer Institute, Villigen	13	2	15	[Bar chart showing 15 total contributions]								
EMPA, Dübendorf/St. Gallen	25	4	29	[Bar chart showing 29 total contributions]								
Eawag, Dübendorf	6	2	8	[Bar chart showing 8 total contributions]								
UAS (FHNW, HES-SO, ZHAW)	12	0	12	[Bar chart showing 12 total contributions]								
Other Academic Institute in Switzerland	4	2	6	[Bar chart showing 6 total contributions]								
Foreign Universities	12	7	19	[Bar chart showing 19 total contributions]								
Chemical/Pharmaceutical Industry	5	16	21	[Bar chart showing 21 total contributions]								
<b>Grand Total</b>	<b>487</b>	<b>94</b>	<b>582</b>									

As the program of the Fall Meeting is tightly packed and the poster session is quite short, there is never enough time for the participants to interact with each other. Therefore, the SCS board decided to expand the 2017 Fall Meeting to one and a half days and to give more time for one-to-one interactions. The first day of the Fall Meeting will end with a social evening (gathering).

**Save the date for the SCS Fall Meeting 2017 in Bern on August 21–22, 2017!**

[1] 'Die Schweizerische Chemische Gesellschaft in den Jahren 1901–1941', im Auftrag des Vorstandes verfasst von H. Rupe, Archiv SCG.

## PROGRAM OVERVIEW

Interactive program incl. all abstracts of the lectures, talks and posters on <http://scg.ch/fallmeeting>

Time	Program	Lecture hall
09.00	Welcome Coffee Registration and poster installation	Lichthof
09.45	Welcome and conference opening PD Dr. <b>Hans Peter Lüthi</b> , Chair SCS Fall Meeting Prof. <b>Michael Schaepman</b> , Dean of the Faculty of Science, University of Zurich	G30
09.55	Invited Lecture as SCS Honorary Member 2016 Prof. <b>E. Peter Kündig</b> «Whole New Landscapes» [PS-001]	G30
10.30	Sandmeyer Award Lecture 2016 Dr. <b>Martin Weibel</b> , Dr. <b>Robert Flatt</b> , Dr. <b>Hendrik Heinz</b> , Sika Technology AG «Development of commercial organic additives for the grinding of inorganic solids» [PS-002]	G30
11.15	<b>Morning Parallel Session (6 or 7 Slots)</b> Analytical Sciences [AS-011] ... [AS-016] Catalysis Science & Engineering [CE-011] ... [CE-017] Computational Chemistry [CC-011] ... [CC-016] Inorganic & Coordination Chemistry [IC-011] ... [IC-016] Medicinal Chemistry & Chemical Biology [MC-011] ... [MC-016] Organic Chemistry [OC-011] ... [OC-016] Physical Chemistry [PC-011] ... [PC-016] Polymers, Colloids & Interfaces [PI-011] ... [PI-016]	G95 G20 G91 G30 G19 G45 G40 G55
12.45	Lunch and <b>Poster Session</b> Analytical Sciences [AS-101] ... [AS-154] Catalysis Science & Engineering [CE-101] ... [CE-162] Computational Chemistry [CC-101] ... [CC-133] Inorganic & Coordination Chemistry [IC-101] ... [IC-184] Medicinal Chemistry & Chemical Biology [MC-101] ... [MC-171] Organic Chemistry [OC-102] ... [OC-183] Physical Chemistry [PC-101] ... [PC-153] Polymers, Colloids & Interfaces [PI-101] ... [PI-151] <b>Commercial Exhibition</b>	Lichthof Galleries           Lichthof
15.00	<b>Afternoon Parallel Session (7 Slots)</b> Analytical Sciences [AS-021] ... [AS-027] Catalysis Science & Engineering [CE-021] ... [CE-027] Computational Chemistry [CC-021] ... [CC-027] Inorganic & Coordination Chemistry [IC-021] ... [IC-027] Medicinal Chemistry & Chemical Biology [MC-021] ... [MC-027] Organic Chemistry [OC-021] ... [OC-027] Physical Chemistry [PC-021] ... [PC-027] Polymers, Colloids & Interfaces [PI-021] ... [PI-027]	G95 G20 G91 G30 G19 G45 G40 G55
16.45	Break and coffee/refreshments	Lichthof
17.00	<b>Information about SCS Journals</b> <i>CHIMIA</i> , <i>ChemPubSoc</i> and <i>Helvetica Chimica Acta</i>	G30
17.10	Paracelsus Award Lecture 2016 Prof. <b>Michael Graetzel</b> , École Polytechnique Fédérale de Lausanne, EPFL, «Invention and development of the dye-sensitized solar cells» [PS-003]	G30
18.00	Best Oral Presentation Awards (sponsored by Metrohm) Presented by Dr. Volker Frost, Metrohm AG	G30
18.15	Best Poster Presentation Awards (sponsored by DSM) Presented by Dr. Roman Imhof, DSM Nutritional Products Ltd.	G30
18.30	End of the conference	

## GENERAL INFORMATION

Date: September 15, 2016, 09.00 – 18.30  
 Location: University of Zurich, Irchel-Campus  
 Winterthurerstrasse 190  
 CH-8057 Zurich  
 Website: <http://scg.ch/fallmeeting>

### Chairman

PD Dr. Hans Peter Lüthi  
 Laboratory for Physical Chemistry  
 ETH Zurich  
 Tel. +41 44 632 21 05  
[hans.luethi@phys.chem.ethz.ch](mailto:hans.luethi@phys.chem.ethz.ch)

### On-site Organization

Dr. Ferdinand Wild  
 Chemistry Department  
 University of Zurich  
 Tel. +41 44 635 46 46  
[fwild@aci.unizh.ch](mailto:fwild@aci.unizh.ch)

### Conference Secretariat

Swiss Chemical Society  
 David Spichiger and Sarah Schmitz  
 Haus der Akademien  
 Laupenstrasse 7, Postfach  
 CH-3001 Bern  
 Tel. +41 31 306 92 92  
[info@scg.ch](mailto:info@scg.ch)

### Organizing Committee

#### Core team

- PD Dr. Hans Peter Lüthi, ETH Zurich (Chairman)
- Prof. Christian Bochet, University of Fribourg (DFR-President)
- Prof. Roger Alberto, University of Zurich (co-Chairman)
- Dr. Ferdinand Wild, University of Zurich (site manager)
- David Spichiger, Swiss Chemical Society (SCS Head Office)

#### Analytical Sciences

- PD Dr. Stefan Schürch, University of Bern
- Dr. Hanspeter Andres, METAS

#### Catalysis Science and Engineering

- Prof. Christoph Müller, ETH Zurich

#### Computational Chemistry

- Prof. Jürg Hutter, University of Zurich
- Prof. Markus Reiher, ETH Zurich

#### Inorganic Chemistry

- Prof. Bruno Therrien, University of Neuchâtel
- Prof. Martin Albrecht, University of Bern

#### Medicinal Chemistry and Chemical Biology

- Dr. Yves Auberson, Novartis (Medicinal Chemistry)

#### Organic Chemistry

- Prof. Cristina Nevado, University of Zurich
- Prof. Olivier Baudoin, University of Basel

#### Physical Chemistry

- Prof. Frédéric Merkt, ETH Zurich
- Prof. Stefan Willitsch, University of Basel

#### Polymers, Colloids and Interfaces

- Prof. Markus Niederberger, ETH Zurich
- Prof. Andrei Honciuc, ZHAW Wädenswil

## Admission and 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 (+VAT)

Fees for participants without a presentation

- SCS Members: free of charge
- Non-members: CHF 50.00 (+VAT). Pre-registered participants will get an invoice in advance to avoid waiting time at the check-in desk. Pre-registration is possible until August 23, 2016 on the website.

If attending as a SCS member you must bring your SCS membership card with you! To become a member, please go to <http://scg.ch/membership>.

Pre-registration as a participant is possible until August 23, 2016 on <http://scg.ch/fallmeeting>.

## Interactive Program and Abstract Search

The web tools allow you an easy and interactive planning of your conference day.

Go to the Fall Meeting website or the SCS Conference Tool on <http://chemistrycongresses.ch>, login with your SCS login details and profit from the following functions:

- Interactive program overview with abstract preview
- Quick abstracts display as html file
- pdf-file download of abstracts directly to user's mailbox (only if logged in).
- Extensive search functionality

The screenshot displays the 'Swiss Chemical Society Conference Tool' interface. At the top, it lists features: 'conference registration, abstract submission / editing' and 'online conference programme and abstract catalogue'. The main content area is titled 'Schedule for event - SCS Fall Meeting 2016'. A dropdown menu for 'Organic Chemistry' is open, showing sub-topics like 'Physical Chemistry', 'Analytical Sciences', etc. The main table lists sessions with columns for 'Start Time', 'Topic', 'Room', and 'Session Name'. A detailed abstract preview is visible on the right, showing the title 'Chiral Ruthenium-cyclopentadienyl Complexes as Versatile Catalysts for Enantioselective Transformations' by David Roessli, EPFL Lausanne.

## Coffee Breaks and Lunch

Refreshments will be served before the opening ceremony and during the breaks. Sandwiches and drinks will be served during the lunch break. The morning coffee is sponsored by Büchi AG, Uster.

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

## Connection to the Internet

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

## GENERAL MEETING SPONSORS AND SUPPORTERS

The SCS and the meeting organizers gratefully acknowledge the generous support of its main sponsors. Without their contributions, it would not be possible to organize the event for free for members and for a reasonable entry fee for non-members.

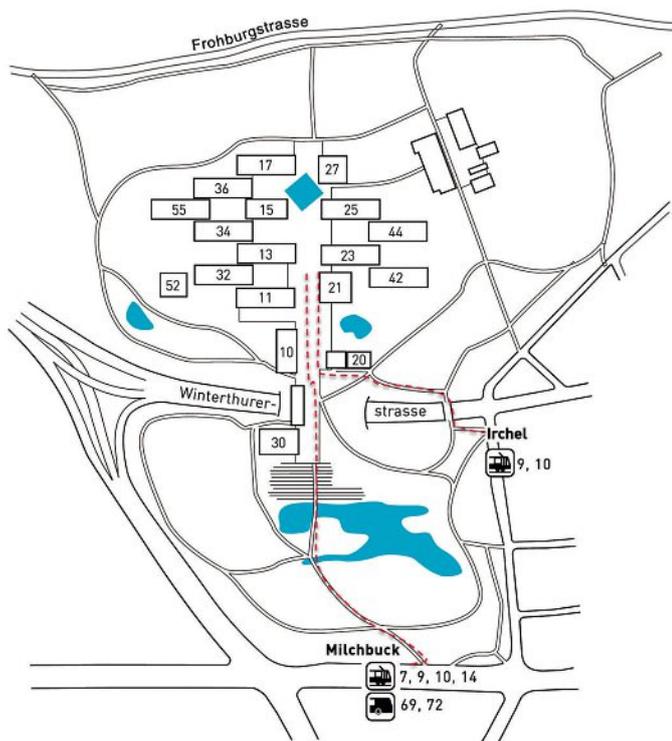


## CONFERENCE VENUE

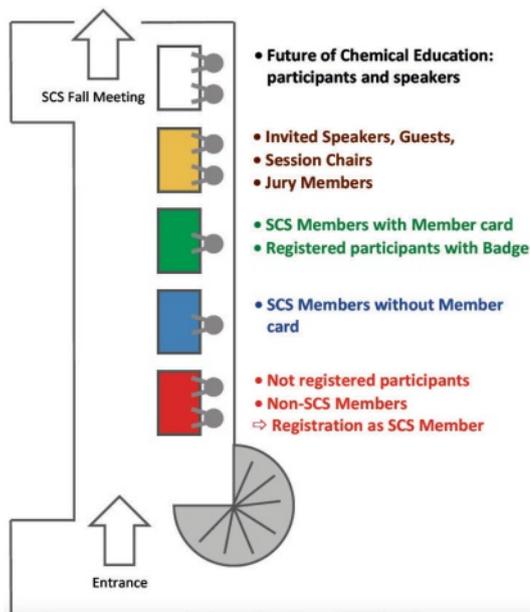
### How to get to the Irchel Campus, University of Zurich

The campus is easily accessible by public transportation. Take tram lines no 9, 10 to Zürich, Universität Irchel or no 7, 14 to Zürich, Milchbuck.

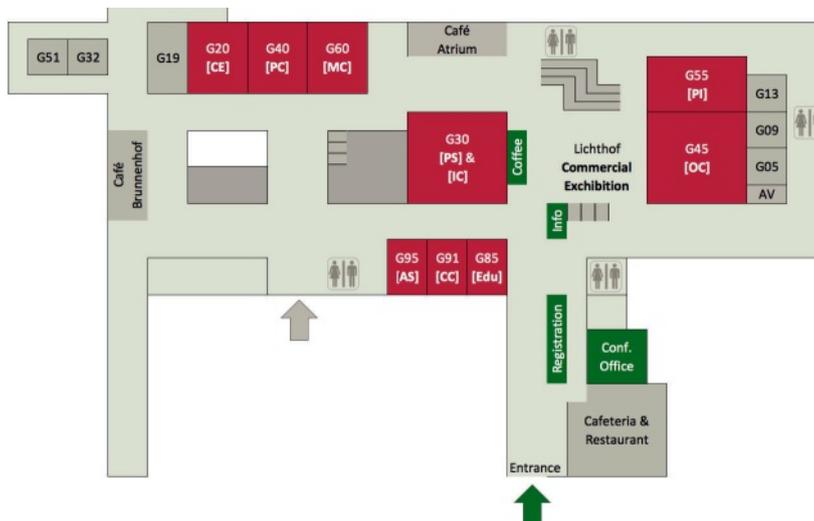
Online schedule on [www.sbb.ch](http://www.sbb.ch)



### Registration



### Site map Irchel Campus



## BEST PRESENTATION AWARDS

The organizers are proud of the very attractive presentation award program. Almost CHF 50'000 CHF in total are given to the winners in monetary form, travel grant or free publication opportunities in the Junior Laureates issue of CHIMIA 4/2017.

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

### Best Oral Presentation Award

The prize is sponsored by Metrohm.



The prize is given for the two best presentations of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation.

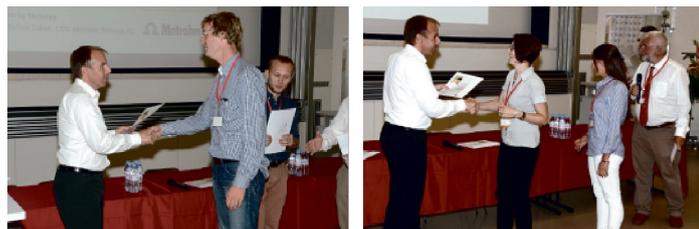
Ceremony: 18.00 in the 'Big Auditorium' (G 30).

### Prizes for the Winner of each Session

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

### Prizes for the Runners-up

- Cash contribution of CHF 400.



Ceremony of the Best Oral Presentation Award at EPFL 2015

### Jury Members Best Oral Presentation Awards

Analytical Sciences (AS)

- Hanspeter Andres, Metas
- Stefan Schürch, University of Bern

Computational Chemistry (CC)

- Ivano Tavernelli, IBM
- Marcella Iannuzzi, University of Zurich

Catalysis Sciences & Engineering

- Christoph Müller, ETH Zurich
- Alexey Fedorov, ETH Zurich
- Aleix Comas Vives, ETH Zurich

Inorganic Chemistry (IC)

- Martin Albrecht, University of Bern
  - Bruno Therrien, University of Neuchatel
- Medicinal Chemistry & Chemical Biology (MC)
- Yves Auberson, Novartis Institutes for BioMedical Research
  - Jean-Louis Reymond, University of Bern

- Georg Jaeschke, F. Hoffmann-La Roche
  - Michele Leuenberger, University of Bern
- Organic Chemistry (OC)

- Cristina Nevado, University of Zurich
  - Olivier Baudoin, University of Basel
- Physical Chemistry (PC)

- Samuel Leutwyler, University of Bern
  - Frédéric Merkt, ETH Zurich
- Polymers, Colloids & Interfaces

- Peter Nesvadba, BASF Schweiz
- Eva-Maria Kupsch, Dow Europe GmbH
- Markus Niederberger, ETH Zurich
- Andrei Honciuc, Zurich University of Applied Sciences

### Best Poster Presentation Award

The prize is sponsored by DSM.



The prizes were given for the best posters of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation.

Ceremony: 18.15 in the 'Big Auditorium' (G 30).

### Prize for the Winner of each Session

- Cash contribution of CHF 500.
- Travel voucher of CHF 750 to attend an international conference.

### Prize for the Runners-up

- 1× runner-up prize for Computational Chemistry
  - 2× runner-up prizes for all other Sessions
- Cash contribution of CHF 300.



Ceremony of the Best Poster Presentation Award at EPFL 2015

### Jury Members Best Poster Presentation Awards

Analytical Sciences (AS)

- Hanspeter Andres, Metas
- Stefan Schürch, University of Bern

Computational Chemistry (CC)

- Erich Wimmer, Materials Design
- Christoph Taeschler, Lonza

Catalysis Sciences & Engineering

- Christoph Müller, ETH Zurich
- Alexey Fedorov, ETH Zurich
- Aleix Comas Vives, ETH Zurich

- Igor V. Koptuyug (Novosibirsk)

- José Rodriguez (Brookhaven)

Inorganic Chemistry (IC)

- Paul J. Dyson, EPF Lausanne
- Fabio Zobi, University of Fribourg
- Julien Furrer, University of Bern

- Martin Albrecht, University of Bern

- Bruno Therrien, University of Neuchatel

Medicinal Chemistry & Chemical Biology (MC)

- Yves Auberson, Novartis Institutes for BioMedical Research

- Jean-Louis Reymond, University of Bern

- Georg Jaeschke, F. Hoffmann-La Roche

- Michele Leuenberger, University of Bern

Organic Chemistry (OC)

- Andreas Herrmann, Firmenich
- Tomas Smejkal, Syngenta Crop Protection
- Cristina Nevado, University of Zurich

- Olivier Baudoin, University of Basel

Physical Chemistry (PC)

- Hans-Jakob Wörner, ETH Zurich
- Jacques-Edouard Moser, EPF Lausanne
- Natalie Banerji, University of Fribourg

- Peter Nesvadba, BASF Schweiz

- Eva-Maria Kupsch, Dow Europe GmbH

- Markus Niederberger, ETH Zurich

- Andrei Honciuc, Zurich University of Applied Sciences

## SPONSORS AND ENDOWMENTS

### Givaudan Suisse SA Endowment of the Plenary Session



As the world's foremost fragrances and flavors business, Givaudan creates products that truly engage the senses, through innovating exquisite aromas and delicious tastes. Headquartered in Switzerland, Givaudan sources and develops ingredients for thousands of its customers' products and technologies, which are enjoyed every day by consumers around the world. [www.givaudan.com](http://www.givaudan.com)

### Clariant International Ltd Endowment Session Catalysis Sciences & Engineering



As one of the world's leading specialty chemical companies, Clariant contributes to value creation with innovative and sustainable solutions for customers from many industries. Our portfolio is designed to meet very specific needs with as much precision as possible. At the same time, our research and development is focused on addressing the key trends of our time. These include energy efficiency, renewable raw materials, emission free mobility, and conserving finite resources. [www.clariant.com](http://www.clariant.com)

### Materials Design Endowment Session Computational Chemistry



Founded in 1998 by a team of leading scientists, Materials Design® is a company designed for today's world with employees and partners working on three continents and in seven time zones. Not being tied down to one location or one time zone means that there is a continuous work flow. As the sun sets in one part of the world, it rises in another. This gives us a truly global perspective and the agility to respond quickly to our customers no matter where they are in the world. [www.materialsdesign.com](http://www.materialsdesign.com)

### Actelion Ltd. Endowment Session Medicinal Chemistry & Chemical Biology



Actelion Ltd. is a leading biopharmaceutical company focused on the discovery, development and commercialization of innovative drugs for diseases with significant unmet medical needs. The company has its corporate headquarters in Allschwil/Basel, Switzerland where it was founded in 1997. [www.actelion.ch](http://www.actelion.ch)

### Syngenta Crop Protection AG Endowment Session Organic Chemistry Session



Syngenta is one of the world's leading companies with more than 28,000 employees in over 90 countries dedicated to our purpose: Bringing plant potential to life. Through world-class science, global reach and commitment to our customers we help to increase crop productivity, protect the environment and improve health and quality of life. [www.syngenta.com](http://www.syngenta.com)

### Bruker BioSpin Endowment Session Physical Chemistry



Bruker Corporation is the global market and technology leader in analytical magnetic resonance instruments including NMR, preclinical MRI and EPR. The Bruker BioSpin Group of companies develop, manufacture and supply technology to research establishments, commercial enterprises and multi-national corporations across countless industries and fields of expertise. [www.bruker.com](http://www.bruker.com)

### Dow Europe GmbH Endowment Session Polymers, Colloids & Interfaces



Dow combines the power of science and technology to passionately innovate what is essential to human progress. The Company is driving innovations that extract value from the intersection of chemical, physical and biological sciences to help address many of the world's most challenging problems such as the need for clean water, clean energy generation and conservation, and increasing agricultural productivity. [www.dow.com](http://www.dow.com)

### Contact Group for Research Matters (KGF)

#### General Supporter of the Swiss Chemical Society

The KGF coordinates research

policies and matters of common interest to its member companies. It facilitates the interactions between its member companies and external partners, e.g. individuals or groups at Swiss research institutions, by acting as a homogeneous discussion partner or sounding board, providing harmonized opinions, recommendations, or action plans. [www.kgf.ch](http://www.kgf.ch)



### Metrohm AG Sponsor of the Best Oral Presentation Award



Metrohm AG, 100% owned by Metrohm Foundation, is one of the world's biggest providers of high precision analytical instruments for analytical sciences. The company was founded in 1943 by Ing. Bertold Suhner and is headquartered in Herisau. [www.metrohm.com](http://www.metrohm.com)

### DSM Nutritional Products Ltd. Sponsor of the Best Poster Presentation Award



DSM Nutritional Products is one of the world's leading suppliers of vitamins, carotenoids and other ingredients to the feed, food, pharmaceutical and personal care industries. A fully integrated global player, our business is organized into three market-facing businesses: Animal Nutrition & Health, Human Nutrition & Health and Personal Care. [www.dsm.com](http://www.dsm.com)

### Swiss Academy of Science, Platform Chemistry General Meeting Supporter



The SCNAT reinforces the awareness of sciences as a central foundation for our cultural and economic development. Its wide establishment in the scientific environment enables the SCNAT to be an important and representative partner of the international scientific policy. The SCNAT networks sciences, makes its expertise available, promotes the dialogue between science and society and identifies and assesses the scientific progress to build and reinforce the working base of the next generation of scientists. [www.scnat.ch](http://www.scnat.ch)

### SCS Foundation General Meeting Supporter

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## COMMERCIAL EXHIBITORS

Take the chance and visit our partners during the day and profit from their expertise to answer your questions. The exhibition will be located in the 'Lichthof' of the Irchel Campus, right after the registration and in front of the big auditorium and the coffee/lunch bench.



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## CONFERENCE SUPPORTERS



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Award Lectures  
Overview

- 09.55 **SCS Honorary Member 2016**  
**Prof. E. Peter Kündig,**  
**University of Geneva**  
«Whole New Landscapes»  
Plenary Session [PS-001],  
lecture hall G30.  
The honorary membership is given  
in recognition of Prof. E. Peter Kündig's research  
achievements in organic synthesis and catalysis with  
transition metals and to honor his far-ranging and  
thoughtful management as president of the Platform  
Chemistry of the Academy of Natural Sciences in the  
years 2007–2009 and as president of the Swiss Chemi-  
cal Society in the past 6 years since 2010.
- 
- 10.30 **Sandmeyer Award Lecture 2016**  
**Dr. Martin Weibel, Dr. Robert Flatt, Dr. Hendrik  
Heinz, Sika Technology AG**  
«Development of new commercial organic addi-  
tives for the grinding of inorganic solids»  
Plenary Session [PS-002], lecture hall G30.  
The award is given to the team comprising researchers  
from Sika Technology AG, ETH Zurich and the Uni-  
versity of Colorado Boulder for their experimental and  
modeling studies of new commercial organic additives  
for the grinding of inorganic solids.
- 11.15 **KGF-SCS Senior Industrial  
Science Award Lecture 2016**  
**Dr. Eric Francotte, Novartis  
Pharma AG**  
«Chromatographic resolution  
of racemic compounds on opti-  
cally active polymers as chiral  
stationary phases»  
Session of Analytical Sciences, [AS-011], lecture hall  
G95.  
The award is given for Dr. Francotte's outstanding  
contributions to chromatographic resolution of race-  
mic compounds on optically active polymers as chiral  
stationary phases and his pioneering work in imple-  
menting new preparative chromatographic techniques.
- 
- 11.15 **KGF-SCS Senior Industrial  
Science Award Lecture 2016**  
**Prof. Peter Nesvadba,**  
**BASF Schweiz AG**  
«Radicals in the Life of Indus-  
trial Polymer»,  
Session of Polymers, Colloids &  
Interfaces, [PI-011], lecture hall G55.  
The award is given for Prof. Nesvadba's groundbreak-  
ing contributions to the discovery and development of  
novel stabilizers for monomers and polymers, novel  
dyes, first industrial realization of controlled radical  
polymerization, to the development of safe alternatives  
to organic peroxides and for his engagement as bridge  
builder between academia and industry.
- 

- 11.15 **KGF-SCS Industrial Science  
Award Lecture 2016**  
**Dr. Martin H. Bolli, Actelion  
Pharmaceuticals Ltd**  
«The Discovery of Macitentan  
- A Standard Medicinal Chem-  
istry Approach?»  
Session of Medicinal Chemistry & Chemical Biology  
[MC-012], lecture hall G60.  
The award is given for Dr. Bolli's excellent contribu-  
tions in medicinal chemistry culminating in the dis-  
covery and development of Macitentan, a drug for the  
treatment of pulmonary arterial hypertension.
- 
- 11.15 **KGF-SCS Industrial Science  
Award Lecture 2016**  
**Dr. Andreas Herrmann,**  
**Firmenich SA**  
«Profragrance chemistry  
as interdisciplinary research  
area and key technology for  
fragrance delivery», Session of Organic Chemistry,  
[OC-011], lecture hall G45.  
The award is given for Dr. Herrmann's essential con-  
tributions to make profragrance chemistry an inter-  
disciplinary research area and to establish it as a key  
technology for fragrance delivery.
- 
- 17.00 **Paracelsus Award Lecture 2016**  
**Prof. Michael Graetzel, EPF  
Lausanne**  
«Invention and development of  
the dye-sensitized solar cells»,  
Plenary Lecture, lecture hall G30.  
The award is given for Prof. Graetzel's invention and  
development of the dye-sensitized  
solar cell.
- 

## Plenary Sessions – G30

Chair: Dr. Hans Peter Lüthi,  
Prof. Roger Alberto

Session Endowment: Givaudan Suisse SA

- 09.55 «Whole New Landscapes» (Lecture of the SCS  
Honorary Member 2016) [PS-001]  
Prof. E. Peter Kündig, University of Geneva
- 10.30 **Sandmeyer Award Lecture 2016:** «Develop-  
ment of new commercial organic additives  
for the grinding of inorganic solids» [PS-002]  
Dr. Martin Weibel, Dr. Robert Flatt, Dr. Hendrik Heinz,  
Sika Technology AG
- 17.00 **Paracelsus Award Lecture 2016:** «Invention and de-  
velopment of the dye-sensitized solar cells» [PS-003]  
Prof. Michael Graetzel, EPF Lausanne

## Abstract codes

[PS-001]...[PS-003]	Plenary Lectures
[XY-011]...[XY-019]	Morning session lectures
[XY-021]...[XY-029]	Afternoon session lectures
[XY-101]...[XY-199]	Posters
AS	Analytical Sciences
CC	Computational Chemistry
CE	Catalysis Sciences & Engineering
IC	Inorganic Chemistry
MC	Medicinal Chemistry & Chemical Biology
OC	Organic Chemistry
PC	Physical Chemistry
PI	Polymers Colloids & Interfaces
PS	Plenary Session

## PARALLEL SESSIONS

## Analytical Sciences [AS]

## Morning Session – G95

Chair: Dr. Hanspeter Andres

No Session Endowment

- 11.15 **Chromatographic resolution of racemic compounds on optically active polymers as chiral stationary phases [AS-011]**  
Eric Francotte, Novartis Institutes for Biomedical Research
- 11.45 **Towards a better understanding of spectral similarity between structurally related compounds [AS-013]**  
Jennifer E. Schollée, Eawag, Dübendorf (*J. Hollender*)
- 12.00 **Understanding the cellular distribution and protein targets of a ruthenium (II) anti-cancer compound, RAPTA-T via mass spectrometry [AS-014]**  
Ronald F. S. Lee, EPF Lausanne (*P. J. Dyson*)
- 12.15 **Combined GC- and UHPLC-HR-MS based metabolomics to analyze durable anti-fungal resistance processes in cereals [AS-015]**  
Rahel Bucher, University of Zurich (*B. Keller*)
- 12.30 **Compound-specific isotope analysis of environmental organic micropollutants: challenges and possibilities [AS-016]**  
Rani Bakkour, Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf (*T. Hofstetter*)

## Afternoon Session – G95

Chair: Dr. Stefan Schürch

- 15.15 **Electrochemical Proton Transfer Based Polyaniline Films for Thin Layer Titrations [AS-022]**  
Majid Ghahraman Afshar, University of Geneva (*E. Bakker*)
- 15.30 **Persistent organic pollutants in white-blooded Antarctic fish *Champscephalus gunnari* and *Chaenocephalus aceratus* [AS-023]**  
Markus Zennegg, Empa
- 15.45 **Field-scale *in situ* analysis of ambient N<sub>2</sub>O isotopic composition to trace source processes in an intensively managed grassland [AS-024]**  
Erkan Ibrahim, Empa (*J. Mohn*)
- 16.00 **At the interface between climate research and metrology: Gas adsorption and desorption on high pressure standard cylinders [AS-025]**  
Ece Satar, University of Bern Physics Institute (*H. Andres*)
- 16.15 **Enzyme-Substrate Complexes Studied by Native Electrospray Mass Spectrometry: First Steps Towards Gas-Phase Enzymology [AS-026]**  
Martin Francis Czar, ETH Zurich (*R. Zenobi*)
- 16.30 **Studies on discrete samples using a microdroplet generator combined with ICP-Time-of-Flight Mass Spectrometry [AS-027]**  
Lyndsey Hendriks, ETH Zurich (*D. Günther*)

## Computational Chemistry [CC]

## Morning Session – G91

Chair: Dr. Ivano Tavernelli



Session Endowment: Materials Design

- 11.15 **Industrial Impact of Computational Chemistry and Materials Science [CC-011]**  
Erich Wimmer, Materials Design s.a.r.l.
- 11.45 **Balancing London dispersion and the delocalization error with DFT functionals [CC-013]**  
Alberto Fabrizio, EPF Lausanne (*C. Corminboeuf*)
- 12.00 **A fast scheme for approximated Fock exchange potentials in plane wave implementations of Kohn-Sham Density Functional Theory [CC-014]**  
Martin Bircher, EPF Lausanne (*U. Röthlisberger*)
- 12.15 **Quantitative Reaction Energies from an Automated Multi-Configurational Approach [CC-015]**  
Christopher Stein, ETH Zurich (*M. Reiher*)
- 12.30 **FDE-ADC: Multiscale density embedding with an accurate wavefunction method. [CC-016]**  
Alexander Zech, University of Geneva (*T. A. Wesolowski*)

## Afternoon Session – G91

Chair: Dr. Marcella Iannuzzi

- 15.00 **Industrial modeling aspects of 1,3-dicarbonyl compounds [CC-021]**  
Christoph Taeschler, Lonza AG
- 15.30 **Is oxide hydrogenation equivalent to reduction? Fundamental differences between TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from DFT [CC-023]**  
Clelia Spreafico, ETH Zurich (*J. VandeVondele*)
- 15.45 **Interatomic many-body representation improves molecular machine learning models [CC-024]**  
Bing Huang, University of Basel (*O. Lilienfeld*)
- 16.00 **Reactive Molecular Dynamics and Infrared Spectra of Double Proton Transfers with Coupling Effects [CC-025]**  
Zhen-Hao Xu, University of Basel (*M. Meuwly*)
- 16.15 **On the ultrashort pulse approximation for the interaction of molecule with pulsed laser fields: Generalization of the Franck-Condon principle [CC-026]**  
Aurélien Patoz, EPF Lausanne (*J. Vanicek*)
- 16.30 **Dry Reforming and Competitive Reactions on Ni, Pd and Pt metal Surfaces from DFT Calculations and Microkinetic Modeling Simulations [CC-027]**  
Aleix Comas-Vives, ETH Zurich

**Catalysis Sciences & Engineering [CE]**  
**Morning Session – G20**  
 Chair: Prof. Christoph Müller

**CLARIANT** 

Session Endowment: Clariant International Ltd.

- 11.15 ***In situ* Studies on the Behavior of Metal/Oxide Catalysts during the Water-gas Shift Reaction [CE-011]**  
 José A. Rodriguez, Brookhaven National Laboratory, USA
- 11.45 **Parahydrogen-based hypersensitive NMR/MRI toolkit for catalysis [CE-013]**  
 Igor V. Koptug, International Tomography Center, Novosibirsk, Russia
- 12.15 **A closure to the controversy around hydrogen spillover: a nanolithography and single nanoparticle spectro-microscopy approach [CE-015]**  
 Waiz Karim, ETH Zurich/PSI Villigen (*J. A. van Bokhoven*)
- 12.30 **Photoelectrochemical Water Splitting from Earth-Abundant CuO Thin Film Photocathode: Enhancing Performance and Photo-stability through Deposition of Overlayers [CE-016]**  
 Wilman Septina, University of Zurich (*D. Tiley*)
- 12.45 **Why Size Matters and Favors CO Activation on Larger Ru Nanoparticles: A Molecular Understanding from First Principles [CE-017]**  
 Lucas Foppa, ETH Zurich (*C. Copéret*)

**Afternoon Session – G20**

Chair: Dr. Alexey Fedorov

- 15.00 **Modelling the Phosphorous Dynamics of Vanadyl Pyrophosphate Catalysts [CE-021]**  
 Gerhard Mestl, Clariant Produkte (Deutschland) GmbH
- 15.30 **On purpose CO production via methane oxychlorination over heterogeneous catalysts [CE-023]**  
 Vladimir Paunovic, ETH Zurich (*J. Pérez-Ramírez*)
- 15.45 **Rational design of ceria-based supported noble metal catalysts for low temperature CO oxidation using transient X-ray absorption spectroscopy [CE-024]**  
 René Kopelent, Paul Scherrer Institute, Villigen (*O. V. Safonova*)
- 16.00 **TiO<sub>2</sub> nanocontainers and nanospheres as photocatalysts for CO<sub>2</sub> reduction and photoelectrochemical water splitting: Structural modification [CE-025]**  
 Nelly Héroult, University of Fribourg (*K. M. Fromm*)
- 16.15 **Understanding of the role of Fe in highly active and stable Ni-Fe dry reforming catalysts [CE-026]**  
 Sung Min Kim, ETH Zurich (*C. Müller*)
- 16.30 **Chemical layer deposition of porous alumina overcoats increases activity and stability in liquid phase catalytic conversion of biomass-derived chemicals [CE-027]**  
 Florent Héroguel, EPF Lausanne (*J. Luterbacher*)

**Inorganic & Coordination Chemistry [IC]**  
**Morning Session – G30**  
 Chair: Prof. Martin Albrecht

No Session Endowment

- 11.15 **Natural Born Catalysts: Photocatalytic Water Oxidation by Molecular Metal Oxides [IC-011]**  
 Marcella Bonchio, University of Padova, Italy
- 11.45 **High Oxidation State N-Heterocyclic Carbene Molybdenum Alkylidene Complexes: Functional Group-Tolerant Olefin Metathesis Catalysts [IC-013]**  
 Suman Sen, University of Stuttgart
- 12.00 **Silver(I) N-heterocyclic complexes for C–C bond activation of alkylnitriles and catalytic application in oxazoline synthesis [IC-014]**  
 Rachael Heath, University of Bern (*M. Albrecht*)
- 12.15 **C–H Activations Catalyzed by Transition-Metal Ions Isolated on Metal Oxide Surfaces [IC-015]**  
 Deven Paul Estes, ETH Zurich
- 12.30 **Exploring Trifluoromethylthioethers as ligands – Platinum(II) complexes of 8-(trifluoromethylthio)quinoline [IC-016]**  
 Carl Philipp Rosenau, ETH Zurich (*A. Togni*)

**Afternoon Session – G30**

Chair: Prof. Bruno Therrien

- 15.00 **D-Glucose-Platinum(II) Conjugates for Targeted Delivery of Platinum to Cancer Cells [IC-021]**  
 Malay Patra, Massachusetts Institute of Technology / University of Zurich (*S. J. Lippard*)
- 15.15 **Red-light activated photoCORMs of Mn(I) species bearing symmetric substituted 2,2'-azopyridines [IC-022]**  
 Emmanuel Kottelat, University of Fribourg (*F. Zobi*)
- 15.30 **Not so similar after all. Fundamental differences in reactivity of *fac*-[M(solvent)<sub>3</sub>(CO)<sub>3</sub>]<sup>+</sup> (M = Re, <sup>99</sup>Tc) with CO [IC-023]**  
 Angelo Frei, University of Zurich (*R. Alberto*)
- 15.45 **Controlling architecture of coordination cages via the aspect ratio of the ligands [IC-024]**  
 Suzanne Maria Jansze, EPF Lausanne (*K. Severin*)
- 16.00 **Design Approaches to Blue and White Light Emitting Gold(III) Complexes [IC-025]**  
 Michael Bachmann, University of Zurich (*K. Venkatesan*)
- 16.15 **Anthracene-based ligands for new luminescent coordination polymers [IC-026]**  
 Serhii Vasylevskyi, University of Fribourg (*K. Fromm*)
- 16.30 **Beyond size effects: composition-tunable properties for quaternary Cu-Zn-In-Se quantum dots [IC-027]**  
 Maksym Yarema, ETH Zurich (*V. Wood*)

**Medicinal Chemistry &  
Chemical Biology [MC]  
Morning Session – G60**  
Chair: Dr. Yves Auberson



Session Endowment: Actelion Ltd

- 11.15 **Business Update SCS Division of Medicinal Chemistry and Chemical Biology [MC-011]**  
Yves Auberson, Novartis Pharma AG
- 11.30 **The Discovery of Macitentan – A Standard Medicinal Chemistry Approach? [MC-012]**  
Martin Hans Bolli, Actelion Pharmaceuticals Ltd.
- 11.45 **Deciphering the catalytic mechanism of the sulfoxide synthase EgtB [MC-013]**  
Kristina Goncharenko, University of Basel  
(*F. P. Seebeck*)
- 12.00 **Discovery and Development of the Highly Potent, Highly Selective Cathepsin S Inhibitor RG7625 for the Treatment of Autoimmune Diseases [MC-014]**  
Wolfgang Haap, F. Hoffmann-La Roche AG
- 12.15 **A sticky interaction: Optimizing the hydrophobic stacking between the tyrosine gate of the bacterial lectin FimH with antagonists [MC-015]**  
Brigitte Fiege, University of Basel (*T. Maier*)
- 12.30 **The discovery of a potent and orally available Dot1L inhibitor [MC-016]**  
Frédéric Stauffer, Novartis Pharma AG

**Afternoon Session – G60**  
Chair: Prof. Jean-Louis Reymond

- 15.00 **Optimization of 1,4-Disubstituted Benzodiazepines as Selective and Brain Penetrant Triple Calcium T-Channel Blockers [MC-021]**  
Romain Siegrist, Actelion Pharmaceuticals Ltd.
- 15.15 **A FUC/LecB system to crystallize versatile nucleic acid structures [MC-022]**  
Pascal Röthlisberger, Institut Pasteur (*M. Hollenstein*)
- 15.30 **Synthesis and oomycete fungicidal activity of a new family of inhibitors targeting an oxysterol binding protein [MC-023]**  
Martin Pouliot, Syngenta Crop Protection
- 15.45 **Stereoselective Synthesis and Biological Evaluation of Highly Potent New (–)-Zampanolide Derivatives [MC-024]**  
Tobias Brüttsch, ETH Zurich (*K.-H. Altmann*)
- 16.00 **High Kinetic Stability of T-Hg<sup>II</sup>-T and DNA Polymerase Inhibition [MC-025]**  
Olivia Paula Schmidt, University of Zurich  
(*N. W. Luedtke*)
- 16.15 **Discovery of a Potent and Selective Reversible BTK Inhibitor for the Treatment of Autoimmune Diseases [MC-026]**  
Robert Pulz, Novartis Institutes for Biomedical Research
- 16.30 **Investigations for New Therapeutic Targets for Neurodegenerative Disease. [MC-027]**  
Erika Crane, University of Basel (*K. Gademann*)

**Organic Chemistry [OC]**



**Morning Session – G45**  
Chair: Prof. Cristina Nevado

Session Endowment: Syngenta Crop Protection AG

- 11.15 **Profragrance chemistry as interdisciplinary research area and key technology for fragrance delivery [OC-011]**  
Andreas Herrmann, Firmenich SA
- 11.45 **Helically Chiral Open-Shell Polycyclic Aromatic Hydrocarbons [OC-013]**  
Prince Ravat, University of Basel
- 12.00 **Chiral Ruthenium-cyclopentadienyl Complexes as Versatile Catalysts for Enantioselective Transformations [OC-014]**  
David Kossler, EPF Lausanne
- 12.15 **Inverse Electron-Demand [4 + 2]-Cycloadditions of Ynamides: Access to Novel Pyridine Scaffolds [OC-015]**  
Guillaume Duret, Strasbourg University  
(*N. Blanchard*)
- 12.30 **Stereoselective Arene-Forming Aldol Condensation: Synthesis of Configurationally Stable Oligo-1,2-naphthylenes [OC-016]**  
Dominik Lotter, University of Basel (*C. Sparr*)

**Afternoon Session – G45**  
Chair: Prof. Olivier Baudoin

- 15.00 **Optimization of Manganese Coupling Reaction for Kilogram-scale Preparation of two Aryl-1,3-dione Building Blocks [OC-021]**  
Tomas Smejkal, Syngenta Crop Protection AG
- 15.30 **Mechanosensitive Fluorescent Membrane Probes [OC-023]**  
Quentin Verolet, University of Geneva (*S. Matile*)
- 15.45 **Metal-Catalyzed Stereoselective Dicarbofunctionalization of Alkynes [OC-024]**  
Andrés García-Domínguez, University of Zurich
- 16.00 **Development and applications of C(sp<sup>3</sup>)-H Alkenylation [OC-025]**  
David Dailler, University of Basel (*O. Baudoin*)
- 16.15 **A family of low molecular-weight, organic catalysts for reductive C–C and C–N bond formation [OC-026]**  
Saad Shaaban, University of Vienna (*N. Maulide*)
- 16.30 **Size-controlled nanoparticle formation in aqueous media with a thiol-free tripeptide [OC-027]**  
Stefano Corrà, ETH Zurich

**Physical Chemistry [PC]****Morning Session – G40**

Chair: Prof. Samuel Leutwyler



Session Endowment: Bruker BioSpin

- 11.15 **Time-resolved X-ray absorption spectroscopy indicates a new photodissociation mechanism of dissolved CBr<sub>4</sub> [PC-011]**  
Rok Bohinc, Paul Scherrer Institute  
(*J. A. van Bokhoven*)
- 11.30 **Reaction-detected infrared spectroscopy of state-selected molecular ions [PC-012]**  
Ugo Jacovella, ETH Zurich (*F. Merkt*)
- 11.45 **From non-relativistic pre-Born-Oppenheimer theory to molecular structure [PC-013]**  
Andrea Muolo, ETH Zurich
- 12.00 **Towards hybrid trapping of cold molecules and cold molecular ions [PC-014]**  
Dominik Haas, University of Basel (*S. Willitsch*)
- 12.15 **State-to-state scattering of methane from Ni(111) and epitaxial graphene on Ni(111) [PC-015]**  
Maarten van Reijzen, EPF Lausanne (*R. Beck*)
- 12.30 **Study of the N(4S)+NO(2II) reactive collision at extreme temperatures relevant to the hypersonic flight regime. [PC-016]**  
Otoniel Denis-Alpizar, University of Basel  
(*M. Meuwly*)

**Afternoon Session – G40**

Chair: Prof. Frédéric Merkt

- 15.00 **Spectroscopic separation of <sup>13</sup>C NMR spectra of complex isomeric mixtures by the CSSF-TOCSY-INEPT experiment [PC-021]**  
Aitor Moreno, Bruker BioSpin Corp
- 15.30 **Ultrafast spectroscopy as a tool to investigate the microstructure of donor-acceptor blends for organic photovoltaics [PC-023]**  
Martina Causa, University of Fribourg (*N. Banerji*)
- 15.45 **Surface-Enhanced 2D Attenuated Total Reflectance IR Spectroscopy for Studying Surface-Sensitive Ultrafast Vibrational Dynamics [PC-024]**  
Jan Philip Kraack, University Zurich
- 16.00 **Direct visualization of excited-state symmetry breaking by ultrafast time-resolved infrared spectroscopy [PC-025]**  
Bogdan Dereka, University of Geneva (*E. Vauthey*)
- 16.15 **Rational Design of Nitroxide Biradicals for Efficient Cross-Effect Dynamic Nuclear Polarization [PC-026]**  
Dominik Józef Kubicki, Ecole polytechnique fédérale de Lausanne (*O. Ouari*)
- 16.30 **Microhydration of N1-Cytosine Derivatives [PC-027]**  
Luca Siffert, University of Bern (*S. Leutwyler*)

**Polymers, Colloids & Interfaces [PI]****Morning Session – G55**

Chair: Prof. Markus Niederberger



Session Endowment: Dow Europe GmbH

- 11.15 **Radicals in the Life of Industrial Polymer [PI-011]**  
Peter Nesvadba, BASF Schweiz AG
- 11.45 **Selective attachment of Gold Nanoparticles on Asymmetrically Functionalized Janus Nanoparticles [PI-013]**  
Florian Guignard, Adolphe Merkle Institute - University of Fribourg (*M. Lattuada*)
- 12.00 **Multi-stimuli responsive films designed through layer-by-layer assembly of PAA-b-PNIPAM block copolymers for biomedical applications [PI-014]**  
Alina Osypova, Empa
- 12.15 **Developing New Strategies to study colloidal Nanocrystals using Dynamic Nuclear Polarization NMR Spectroscopy [PI-015]**  
Laura Piveteau, ETH Zurich (*C. Copéret*)
- 12.30 **Combined Electrical and Optical Characterization of Polydiacetylene [PI-016]**  
Clément Girard-Reydet, Université de Genève  
(*K. Sugihara*)

**Afternoon Session – G55**

Chair: Prof. Andrei Honciuc

- 15.00 **Retort tie-layer: the development of a solution for barrier retort structures [PI-021]**  
Eva-Maria Kupsch, Dow Europe GmbH
- 15.30 **Phosphorescent oxygen sensors produced by spot-crazing of polyphenylenesulfide films [PI-023]**  
Claudio Toncelli, Swiss Federal Laboratories for Materials Science and Technology.
- 15.45 **100% Renewables-Based Polyethylene Furanoate (PEF) for the Green Bottle via Ring-Opening Polymerization [PI-024]**  
Jan-Georg Rosenboom, ETH Zurich (*M. Morbidelli*)
- 16.00 **Force-Induced *cis-to-trans* Isomerization of Carbon-Carbon Double Bond Using Atomic Force Microscopy [PI-025]**  
Milad Radiom, University of Geneva (*M. Borkovec*)
- 16.15 **Biomimetic Polymersomes through a Symbiosis of Organic and Polymer Chemistry [PI-026]**  
Jens Gaitzsch, University of Basel (*W. Meier*)
- 16.30 **A novel two-dimensional polymer synthesized by [2+2]-cycloaddition on the multigram scale [PI-027]**  
Ralph Z Lange, ETH Zurich (*A. D. Schlüter*)

## POSTER SESSIONS

### Poster Presentation Title [Code]

First line = Presenting Author

Second line = Coauthors

### Analytical Sciences [AS]

#### Poster Session

**Evidence for laser-induced redox reactions in matrix-assisted laser desorption/ionization between cationizing agents and target plate material: a study with polystyrene and trifluoroacetate salts [AS-101]**

Guido Paul Zeegers, ETH Zurich

R. Steinhoff, S. M. Weidner, R. Zenobi

**Quantifying positional uncertainties in NMR crystallography [AS-102]**

Albert Hofstetter, EPF Lausanne

L. Emsley

**SPRI-MALDI MS: How to follow non-covalent interactions in real time and identify the binding partners directly [AS-103]**

Ulrike Anders, ETH Zurich

F. Hibti, J. Schaefer, C. Frydman, D. Suckau, A. Plückthun, R. Zenobi

**Laser Ablation Time of Flight Mass Spectrometry using Ion Funnel for Trace Element Analysis in Solids [AS-104]**

Lorenzo Querci, ETH Zurich

B. Hattendorf, D. Günther

***In-vivo* mass spectrometric analysis of yeast growth metabolism [AS-105]**

Alberto Tejero, ETH Zurich

D. Garcia Gomez, A. J. Ibanez, P. Martinez-Lozano Sinues, R. Zenobi

**A Laser ablation ICP-TOFMS setup with a 213 nm Laser for High-Resolution, High-Speed and Multielemental Imaging of Biological Tissues [AS-106]**

Gunnar Schwarz, ETH Zurich

J. Koch, B. Hattendorf, D. Günther

**Investigation of the  $^{85}\text{Rb}^+$ - $^{88}\text{Sr}^+$  Signal Separation by Online Electrothermal Vaporization in a fs-LA-ETV-SCICPMS Set-Up [AS-107]**

Hale Ceren Yilmaz, ETH Zurich

B. Hattendorf

**A new twist to current understanding of pollen-induced asthma – non-allergenic, secondary metabolites in pollen induce non-inflammatory airways constriction? [AS-108]**

Alen Bozicevic, University of Basel

M. DeMieri, C. Nassenstein, M. Hamburger

**Characterization of Membrane Proteins and their Complexes by High-Mass Matrix-Assisted Laser Desorption Ionization-Mass Spectrometry [AS-109]**

Martin Köhler, ETH Zurich

C. Perez, K. Locher, R. Zenobi

**Response factor determination of oligomeric proteins in native ESI-MS [AS-110]**

Katharina Root, ETH Zurich

R. Zenobi

**ICP-TOFMS analysis of transient signals generated by laser ablation [AS-111]**

Marcel Burger, ETH Zurich

A. Gundlach-Graham, G. Schwarz, D. Käser, J. Käslin,

B. Hattendorf, D. Günther

**Small-drugs quantification from whole-blood within paper-based microstructures for Point-of-Care Therapeutic Drug Monitoring [AS-112]**

Elena-Diana Burghilea, University of Applied Sciences Western Switzerland

D. Prim, M. Pfeifer, J.-M. Segura

**LA-ICP-MS for quantification of minerals using matrix-matched glasses as external standards [AS-113]**

Debora Käser, ETH Zurich

D. Günther

**Observation of forbidden vibrational transitions in a plasmonic nanogap [AS-114]**

Jacek Szczerbiński, ETH Zurich

L. Opilik, R. Zenobi

**Nanoscale molecular orientation mapping by Tip-Enhanced Raman Spectroscopy [AS-115]**

Feng Shao, ETH Zurich

V. Müller, A. D. Schlüter, R. Zenobi

**Constant Potential Coulometry for All-Solid-State Chloride-Selective Electrodes [AS-116]**

Zdenka Jarolímová, University of Geneva

U. Vanamo, E. Hupa, E. Bakker, J. Bobacka

**Ionization Mechanism of Perfluorinated Compounds Using an Active Capillary Plasma Ionization Source [AS-117]**

Luzia Gyr, ETH Zurich

R. Zenobi

**UV-fs-LA-ICP-TOF-MS for the quantitative analysis of  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  PLD thin films in high spatial resolution [AS-118]**

Kevin Guex, ETH Zurich

J. Koch, D. Günther

**Capillary Gap Sampler: a new microfluidic platform directly coupled to ESI-MS for fast analysis of low sample amounts [AS-119]**

Sahar Ghiasikhou, ETH Zurich

Y. Zhu, R. Zenobi

**Study of the Interaction Between p53 and DNA by Tip-Enhanced Raman Spectroscopy [AS-120]**

Liqing Zheng, ETH Zurich

**Sample Acidification for Potentiometric Sensing of Anions in Environmental Samples [AS-121]**

Nadezda Pankratova, University of Geneva

G. A. Crespo, M. G. Afshar, M. Cuartero, D. Yuan, E. Bakker

**Source apportionment of atmospheric mercury species measured at the high-alpine site Jungfraujoch [AS-122]**

Liviana Klein, ETH Zurich

B. Denzler, C. Bogdal, K. Hungerbühler

**Gas-phase properties of natural and modified nucleic acid duplexes [AS-123]**

Yvonne Hari, University of Bern  
A. Istrate, E. Laczko, C. Leumann, S. Schürch

**Interaction of Metallocenes with Nucleic Acids [AS-124]**

Rahel Eberle, University of Bern  
S. Schürch

**Solid Contact Thin Layer Ionophore Based Membranes for Ion Activity Detection: Two sensing modes [AS-125]**

Dajing Yuan, University of Geneva  
M. Cuartero, G. A. Crespo, E. Bakker

**Mobile spectroscopic real-time monitoring of NO<sub>2</sub> for pollution maps of Zurich [AS-126]**

Morten Hundt, Empa Materials Science and Technology  
M. Müller, M. Mangold, B. Tuzson, C. Hüglin, H. Looser,  
P. Scheidegger, L. Emmenegger

**Polyurethane Thin Layer Membranes for Multiion Detection in Blood and Serum [AS-127]**

Maria Cuartero, University of Geneva  
G. A. Crespo, E. Bakker

**Silver nanoparticle transformations in lake water explored by an asymmetrical flow field-flow fractionation and single particle ICP-MS characterization [AS-128]**

Vera Slaveykova, University of Geneva  
J. Jiménez-Lamana

**Two-dimensional algal array combining AC-dielectrophoresis with ROS fluorescence detection as a contaminant biosensing chip [AS-129]**

Coralie Susillon, University of Geneva  
V. Slaveykova, O. D. Velev

**Mathematical demodulation of interreflection based multi-modulation artefacts in Fourier transform infrared spectroscopy [AS-130]**

Mathias Schilling, Zurich University of Applied Sciences, ZHAW  
J. Stohner

**Proteomics techniques to follow decay of extracellular enzymes in the aquatic environment [AS-131]**

Elisabeth M. Janssen, Eawag, Dübendorf  
C. Egli

**Implementing Plasma-based Extreme UV radiation for table-top nano-analytics [AS-132]**

Davide Bleiner, Empa Materials & Technology  
C. Cirelli, Y. Arbelo Pena, F. Barbato, B. D. Patterson,  
G. R. Patzke

**SOLUTIONS for effective Non-target Screening in environmental samples [AS-133]**

Emma L. Schymanski, Eawag, Dübendorf  
C. Ruttkies, N. Munz, S. Neumann, J. Hollender

**Solvent-based Selective Titration Reagents for High Affinity Complexometric Titrations [AS-134]**

Jingying Zhai, University of Geneva  
E. Bakker

**New SI-traceable reference gas mixtures for sulfur hexafluoride (SF<sub>6</sub>) at the pmol/mol level [AS-135]**

Simon A. Wyss, EMPA, Dübendorf  
S. Reimann, M. Vicar, M. K. Vollmer, C. Pascale, G. Nieuwenkamp, S. Reimann, B. Niederhauser, L. Emmenegger

**Nucleotide and nucleotide sugar quantification in cell extracts by capillary electrophoresis [AS-136]**

Blanka Bucsellà, HES-SO Valais-Wallis  
A. Fornage, D. Brühlmann, F. Kálmán

**Novel instrumentation for analysis of halogenated trace gases by GC-TOFMS (APRECON) [AS-137]**

Benjamin Spenger, EMPA, Dübendorf  
M. K. Vollmer, M. Hill, S. A. Wyss, L. Emmenegger,  
S. Reimann

**Table-top pseudo-spark XUV source for energy dispersive absorption spectroscopy [AS-138]**

Francesco Barbato, Empa Materials & Technology  
C. Cirelli, B. D. Patterson, D. Bleiner

**A novel analytical peak fitting tool for the integration of very noisy or overlapped peaks (for the inexperienced users) [AS-139]**

Manuel R. Mazenauer, Zurich University of Applied Sciences, ZHAW  
C. Yeretzyan

**Can We Use Targeted Proteomics to Explore Dynamics in Glutathione S-Transferase Expression in Zebrafish Embryos? [AS-140]**

Alena Tierbach, Eawag, Dübendorf  
K. Groh, K. Schirmer, M. Suter

**Table-top XUV mass spectrometry for nano-scale chemical imaging [AS-141]**

Yunieski A. Pena, Empa Materials & Technology  
M. Ruiz, C. Cirelli, D. Bleiner

**Distribution and speciation of Ag, Ce and Ti in natural freshwaters [AS-142]**

Flavio Piccapietra, Eawag, Dübendorf  
A. Hofacker, L. Sigg, R. Behra

**Deconvolution of chlorinated paraffins and their transformation products from DI-CE-APCI-qTOF mass spectra [AS-143]**

Lena Schinkel, Empa Materials Science and Technology  
S. Lehner, P. Lienemann, C. Bogdal, K. McNeill, N. Heeb

**Biotransformation of chlorinated paraffins with LinA, a HCH-converting bacterial enzyme found in various *Sphingomonadacea* [AS-144]**

Simone Schalles, Empa Materials Science and Technology  
S. Lehner, L. Schinkel, I. Schilling, N. Heeb, C. Bogdal,  
P. Lienemann, K. McNeill, H. E. Kohler

**Tracking biotransformation of hexachlorocyclohexane isomers by compound-specific isotope analysis [AS-145]**

Iris Schilling, ETH Zurich  
T. Hofstetter, H. E. Kohler

**The Swiss Army Knife of Analytics for Energy Storage [AS-146]**

Andreas Borgschulte, Empa Materials Science and Technology  
D. Bleiner

**Soft X-ray HEROS on photoactive materials [AS-147]**

Claudio Cirelli, Empa Materials Science and Technology  
F. Barbato, Y. Arbelo Pena, A. Borgschulte, L. Mewes,  
D. Kinschel, C. Arrell, J. Budarz, D. Leuenberger,  
B. D. Patterson, M. Chergui, D. Bleiner

**Table-top pseudo-spark XUV source for energy dispersive absorption spectroscopy [AS-148]**

Francesco Barbato, Empa Materials Science and Technology  
C. Cirelli, B. D. Patterson, D. Bleiner

**Gaining a Comprehensive Picture of Transformation Products formed during Wastewater Treatment Processes [AS-149]**

Jennifer E. Schollée, Eawag, Dübendorf  
E. L. Schymanski, M. Bourgin, S. E. Avak, R. Teichler,  
C. S. McArdell, J. Hollender

**A computational workflow for elucidating phytoplankton biotransformation using LC-HRMS [AS-150]**

Michael A. Stravs, Eawag, Dübendorf  
F. Pomati, J. Hollender

**Quantitative Atomistic Simulations of Solute Intercalation in Reversed Phase Liquid Chromatography [AS-152]**

Krystel El Hage, University of Basel  
M. Meuwly

**Advanced Trace Analysis Bridging Industrial & Scientific Challenges [AS-154]**

Renato Figi, Empa Materials Science and Technology  
C. Schreiner, M. Bürki, O. Nagel, H. Hagedorfer,  
Y. Romanyuk, P. Wäger, A. N. Tiwari, D. Bleiner

**Computational Chemistry [CC]  
Poster Session**

**Machine learning energies of 2M elpasolite (ABC2D6) crystals [CC-101]**

Felix Faber, University of Basel  
A. Lindmaa, O. A. von Lilienfeld, R. Armiento

**GW with Gaussian basis functions in CP2K [CC-102]**

Jan Wilhelm, University of Zurich  
J. Hutter

**Structure-function based screening discovers agonists for a prototypical olfactory receptor [CC-103]**

Shuguang Yuan, EPF Lausanne  
T. Dahoun, H. Vogel

**Potential Energy Surface-Based Conformational Analysis: Automatic Deduction of Conformational Reaction Route Maps at the Quantum Mechanical Level [CC-104]**

Hiroko Satoh, University of Zurich  
T. Oda, K. Nakakoji, T. Uno, H. Tanaka, S. Iwata, K. Ohno

**Protein-ligand Interaction Fingerprints of the  $\beta_2$ -Adrenergic Receptor [CC-105]**

H. C. Stephen Chan, University of Bradford  
S. Yuan

**Junction Control: Modulating Conductance Channel and Length Dependence on Molecular Level [CC-106]**

Ganna Gryn'ova, EPF Lausanne  
P. J. Ollitrault, C. Corminboeuf

**Multiscale Analysis for Field-Effect Penetration through 2D Materials [CC-107]**

Tian Tian, ETH Zurich  
C. Shih

**Low-Lying  $\pi\pi^*$  States of Heteroaromatic Molecules: A Challenge for Excited State Methods [CC-108]**

Antonio Prlj, EPF Lausanne  
C. Corminboeuf

**DORI on the move [CC-109]**

Laurent Vannay, EPF Lausanne  
R. Petraglia, C. Corminboeuf

**Mechanistic Study of Denitrification Reaction in Truncated Hemoglobin using Adiabatic Reactive Molecular Dynamics [CC-110]**

Akshaya Kumar Das, University of Basel  
T. Nagy, M. Meuwly

**Modelling the  $\pi$  conjugation length in aromatic antenna: A simple predictive tool for the synthesis of functional material [CC-111]**

Marie Humbert-Droz, University of Geneva  
C. Piguet, T. A. Wesolowski

**Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation [CC-112]**

Mauro Schilling, University of Zurich  
G. R. Patzke, S. Luber, J. Hutter

**Theoretical Investigation on the Nature of Xe Migration in Truncated Hemoglobin N [CC-113]**

Polydefkis Diamantis, University of Basel  
O. Unke, M. Meuwly

**Replacing Porphyrins with Pyrphyrins: Adsorption and Metalation on Au(111) [CC-114]**

Yeliz Gurdal, University of Zurich  
G. Mette, D. Sutter, S. Schnidrig, B. Probst, M. Iannuzzi,  
J. Hutter, R. Alberto, J. Osterwalder, G. Mette

**Exploiting A Tactic for Tuning the Plasmonic Properties of Thiophene Derivatives [CC-115]**

Jian-Hao Li, EPF Lausanne  
C. Corminboeuf

**Benzonitrile as a Potent and Sensitive Spectroscopic Probe for Protein Interiors [CC-116]**

Padmabati Mondal, University of Basel  
P.-A. Cazade, M. Meuwly

**Improving the exploration of free energy landscapes at the electronic structure levels [CC-117]**

Stepan Ruzicka, EPF Lausanne  
R. Petraglia, C. Corminboeuf

**A potential model for molecular dynamics simulations in organic-inorganic halide perovskites [CC-118]**

Ariadni Boziki, EPF Lausanne  
N. A. Astani, S. Meloni, U. Röthlisberger

**Quantum Molecular Dynamics and Cryogenic Spectroscopy Determine the Structure of Cyclic Intermediates Involved in Peptide Sequence Scrambling [CC-119]**

Marta Da Silva Perez, EPF Lausanne  
O. Aseev, T. Rizzo, T. R. Rizzo, U. Röthlisberger

**Rigorous approach to the cellularization of the Herman-Kluk semiclassical propagator [CC-120]**

Sergey Antipov, EPF Lausanne  
J. Vanicek

**Quantum chemistry meets kinetic modeling: Predicting the evolution of chemical processes occurring on multiple time scales [CC-121]**

Jonny Proppe, ETH Zurich  
M. Reiher

**Accelerating equilibrium isotope effect calculations by stochastic integration with respect to mass[1] [CC-122]**

Konstantin Karandashev, EPF Lausanne  
J. Vanicek

**Computational Rationalization of the selectivity of Ru(II) and Os(II) anticancer agents in HIS/HER binding to the histone components of the Nucleosome Core Particle [CC-123]**

Thibaud von Erlach, EPF Lausanne  
C. A. Davey, P. Dyson, U. Röthlisberger

**Targeting Multiple Reactions by Protein Engineering: Hydration of CO<sub>2</sub> and Tetrazole Formation [CC-124]**

Esra Bozkurt, EPF Lausanne  
R. Hovius, T. A. Soares, U. Röthlisberger

**DFT studies on a well-defined Re-oxo complex grafted on Al-modified silica active in olefin metathesis [CC-125]**

Erwin Lam, ETH Zurich  
M. Valla, A. Comas-Vives, C. Copéret

**Exploration of Complex Chemical Reaction Mechanisms [CC-126]**

Gregor Nils Simm, ETH Zurich  
T. Husch, F. Krausbeck, J. Proppe, A. C. Vaucher, M. Reiher

**Integral evaluation of contracted solid harmonic Gaussian functions [CC-127]**

Dorothea Golze, University of Zurich  
N. Benedikter, M. Iannuzzi, J. Hutter

**Second Generation Car-Parrinello MD: Application to supported nanostructures [CC-128]**

Marcella Iannuzzi-Mauri, University of Zurich  
S. Caravati

**Frozen-density embedding theory with average solvent charge densities from explicit atomistic simulations [CC-129]**

Emilie Chalaye-Chemineau, University of Geneva  
A. Laktionov, T. A. Wesolowski

**Influence of empirical van der Waals dispersion correction on the DFT description of alkaline-earth fluorohalides [CC-130]**

Daniel Sethio, University of Geneva  
H. Hagemann, A. Hauser

**Spin crossover in mixed [Co(bpy)<sub>3</sub>][Li<sub>x</sub>Na<sub>1-x</sub>Cr(ox)<sub>3</sub>] crystals [CC-131]**

Missana Andrea, University of Geneva  
L. Daku, A. Hauser

**Computational Study of the Quantum Dynamics of Tunneling and Electroweak Parity Violation in 1,2-dithiine [CC-132]**

Csaba Fábri, ETH Zurich  
L. Horný, M. Quack

**As if They Were Transition Metal Compounds: the Amazing Electronic Structure and Reactivity of Hypervalent Iodine Reagents [CC-133]**

Halua Pinto de Magalhães, ETH Zurich  
O. Sala, A. Togni, H. P. Lüthi

**Catalysis Sciences & Engineering [CE] Poster Session**

**Enhancing the stability of Pd catalysts for methane oxidation using hierarchical ZSM-5 [CE-101]**

Andrey W. Petrov, Paul Scherrer Institut  
D. Ferri, O. Kröcher, J. A. van Bokhoven

**Growth mechanism and optimization of the Co<sub>3</sub>O<sub>4</sub> spinel matrix for water oxidation [CE-102]**

Lukas Reith, University of Zurich  
K. Lienau, R. Moré, D. Cook, R. Walton, Y. Wu, G. R. Patzke

**Controlling particle size distribution of nickel particles supported on  $\gamma$ -alumina by a molecular approach [CE-103]**

Tigran Margossian, ETH Zurich  
K. Larmier, S. Kim, A. Fedorov, C. Copéret, C. Müller

**Ethene-to-Propene Conversion on Well-Defined Surface Nickel Sites [CE-104]**

Iliia Moroz, ETH Zurich  
A. Fedorov, C. Copéret

**Microbial fuel cell triple stack characteristics [CE-105]**

Marc Sugnaux, HES-SO Valais  
C. Savy, G. Huguenin, F. Fischer

**Modeling of Sustainable Base Production by Microbial Electrolysis Cell [CE-106]**

Maxime Blatter, HES-SO Valais  
M. Sugnaux, C. Comninellis, K. Neelson, F. Fischer

**Heterogeneous Catalytic Reactor for H<sub>2</sub> Production from Formic Acid for Use in PEM Fuel Cells [CE-107]**

Igor Yuranov, EPF Lausanne  
A. F. Dalebrook, G. Laurenczy

**Systematic Modeling and Validation of Long-term Waste Incineration Planning in Integrated Chemical Sites [CE-108]**

Teresa P. R. Hernández, ETH Zurich  
V. M. Bolis, M. L. Abächerli, E. Capón-García, K. Hungerbühler

**Sub-nanometre gold particles catalyse transfer hydrogenation of N-heterocyclic compounds [CE-109]**

Beáta Vilhanová, Paul Scherrer Institute  
M. Ranocchiari, J. A. van Bokhoven

**A novel strategy of activating hematite photoanodes for solar water oxidation [CE-110]**

Chunhua Cui, University of Zurich

**The Mechanism of Catalytic Fast Pyrolysis [CE-111]**

Victoria Custodis, ETH Zurich  
P. Hemberger, J. A. van Bokhoven

**Structural Characterization of Sn Sites in Sn-Chabazite by Dynamic Nuclear Polarization Enhanced Solid-State NMR [CE-112]**

Ta-Chung Ong, ETH Zurich  
W.-C. Liao, A. Comas-Vives, J. W. Harris, R. Gounder, C. Copéret

**Mechanistic Insights for Propane Dehydrogenation and Propene Hydrogenation on Cr(III) Aluminates and Cr(III) Silicates [CE-113]**

Murielle F. Delley, ETH Zurich  
D. P. Estes, K. V. Kovtunov, I. V. Koptuyug, C. Copéret

**Dry-reforming of methane over bimetallic Ni-M/La<sub>2</sub>O<sub>3</sub> (M = Co, Fe): The effect of the rate of La<sub>2</sub>O<sub>3</sub>CO<sub>3</sub> formation and phase stability on the catalytic activity and stability [CE-114]**

Athanasia Tsoukalou, ETH Zurich  
Q. Imtiaz, S. Kim, P. M. Abdala, S. Yoon, C. Müller

**Cationic Silica-Supported N-Heterocyclic Carbene Tungsten Oxo Alkylidene Sites: Highly Active and Stable Catalysts for Olefin Metathesis [CE-115]**

Margherita Pucino, ETH Zurich  
V. Mougel, A. Fedorov, C. Copéret

**Sulfur on nickel catalysts impedes the desorption of reaction products [CE-116]**

Jasmin Terreni, Empa Materials Science and Technology  
D. Bleiner, A. Borgschulte

**Reaction intermediates and pathways for CO<sub>2</sub> hydrogenation on Cu/ZrO<sub>2</sub> catalysts: a combined DFT and experimental approach [CE-117]**

Kim Larmier, ETH Zurich  
S. Tada, A. Comas-Vives, W.-C. Liao, C. Copéret

**Synthesis of mordenite with targeted aluminum site distribution using structure directing agents [CE-118]**

Amy Knorpp, ETH Zurich  
A. Pinar, M. Ranocchiari, J. A. van Bokhoven

**Methane Activation: Transformation to Ethylene, Aromatics and Other Species [CE-119]**

Petr Sot, ETH Zurich  
C. Copéret, J. A. van Bokhoven

**Structure analysis of Zn-DAF-1 [CE-120]**

Ana Pinar, Paul Scherrer Institut  
L. McCusker

**Effect of noble metal nanoparticles on the conduction band electrons in UV-excited titania nanocrystallites for photocatalytic applications [CE-121]**

Arno Schneider, ETH Zurich/PSI Villigen  
J. A. van Bokhoven

**Computational investigation and design of biomimetic cubane water oxidation catalysts [CE-122]**

Sandra Luber, University of Zurich  
F. Hodel

**Catalyst and process design for glycerol valorization to commodities [CE-123]**

Giacomo Marco Lari, ETH Zurich  
C. Mondelli, J. Pérez-Ramírez

**Improved numerical methods for the characterization of zeolite catalysts by positron annihilation spectroscopy [CE-124]**

Asier Zubiaga, ETH Zurich  
R. Warringham, S. Mitchell, P. Crivelli, J. Pérez-Ramírez

**Catalyst and process design for the preparation of sugar alcohols by epimerization-hydrogenation [CE-125]**

Giacomo Marco Lari, ETH Zurich  
O. Gröninger, C. Mondelli, J. Pérez-Ramírez

**Enhanced electrocatalytic reduction of CO<sub>2</sub> to CO over Cu-based composites: catalyst equilibration is the key [CE-126]**

Gastón O. Larrazábal, ETH Zurich  
A. J. Martín-Fernández, J. Pérez-Ramírez

**Sustainable polyurethane raw materials through heterogeneous aluminosilicate catalysts: From active site quality to reactor design [CE-127]**

Tobias Keller, ETH Zurich  
M. O. Haus, J. Arras, J. Pérez-Ramírez

**Stabilization of catalytically-active metal atoms on graphitic carbon nitride [CE-128]**

Evgeniya Vorobyeva, ETH Zurich  
Z. Chem, P. Midgley, R. Leary, J. Meurig Thomas, N. López, G. Vilé, S. Mitchell, J. Pérez-Ramírez

**Catalytic oxidation of ethanol to acetic acid in liquid flow [CE-129]**

Sotiria Mostrou, ETH Zurich  
T. Sipócz, L. Kocsis, R. V. Jones, F. Darvas, J. A. van Bokhoven

**Higher alcohol synthesis over modified Fischer-Tropsch catalysts [CE-130]**

Ho T. Luk, ETH Zurich  
C. Mondelli, D. Curulla-Ferré, J. A. Stewart, J. Pérez-Ramírez

**The cascade solution: solid base catalysts for the intermediate deoxygenation of bio-oil *via* aldol condensation [CE-131]**

Tobias C. Keller, ETH Zurich  
B. Puertolas, J. Pérez-Ramírez

**Glucose-derived platform chemicals *via* zeolite-catalyzed fast pyrolysis [CE-132]**

Begona Puertolas, ETH Zurich  
Q. Imtiaz, C. R. Müller, J. Pérez-Ramírez

**Exploiting the reversible segregation of Ni in redox stable La-Fe-Ni catalysts [CE-133]**

Patrick Steiger, Paul Scherrer Institut  
O. Kröcher, D. Ferri

**Structuring hybrid Pd nanoparticles in metallic monolith channels for superior alkyne semi-hydrogenation performance in flow [CE-134]**

Davide Albani, ETH Zurich  
G. Vilé, S. Mitchell, J. Pérez-Ramírez

**Triazolium-based ionic liquids for electrochemical reduction of CO<sub>2</sub> [CE-135]**

Dmitry Vasilyev, EPF Lausanne  
P. Dyson

**Structure-performance relations in the semi-hydrogenation of acetylene over indium oxide [CE-136]**

Davide Albani, ETH Zurich  
O. Martin, G. Vilé, S. Mitchell, N. López, J. Pérez-Ramírez

**The Significance of Lewis Acid Sites for the Selective Catalytic Reduction of Nitric Oxide on Vanadium-Based Catalysts [CE-137]**

Adrian Marberger, Paul Scherrer Institut, Villigen  
D. Ferri, M. Elsener, O. Kröcher

**Controlling the selectivity to chemicals from lignin *via* catalytic fast pyrolysis [CE-138]**

Zhiqiang Ma, ETH Zurich  
V. Custodis, A. Ghosh, J. A. van Bokhoven

**Quantifying the complex pore architecture of hierarchical faujasite zeolites and the impact on diffusion [CE-139]**

Robbie Warringham, ETH Zurich  
T. C. Keller, P. Crivelli, J. Kenvin, M. Sterling, J. J. S. Mitchell, J. Pérez-Ramírez

**Monitoring pore evolution during the detemplation of zeolite catalysts by positron annihilation spectroscopy [CE-140]**

Robbie Warringham, ETH Zurich  
A. Zubiaga, L. Gerchow, P. Crivelli, S. Mitchell, J. Pérez-Ramírez

**CO activation on supported Pt single-atom catalysts: a density functional theory study [CE-141]**  
Xing Wang, ETH Zurich/PSI Villigen  
D. Palagin, J. A. van Bokhoven

**Highly selective and stable copper-zinc catalyst for carbon dioxide hydrogenation of methanol [CE-142]**  
Jin Hee Lee, Paul Scherrer Institute  
S. Saedy, M. Ranocchiari, J. A. van Bokhoven

**Cobalt-Nickel Spinels and Doped Manganese Oxides as Water Oxidation Catalysts [CE-143]**  
Michael Olah, University of Zurich  
G. R. Patzke

**Catalyst design for methane oxyhalogenation – comparison between chlorine and bromine chemistry [CE-144]**  
Guido Zichittella, ETH Zurich  
V. Paunovic, N. Aellen, A.P. Amrute, J. Pérez-Ramírez

**Mechanism of bifunctional ceria in vinyl chloride manufacture from ethylene [CE-145]**  
Matthias Scharfe, ETH Zurich  
M. Capdevila, A.P. Amrute, V. Paunovic, D. Teschner, L. Szentmiklósi, M. Jankowski, J. Drnec, N. López, J. Pérez-Ramírez

**Europium oxide – a highly selective catalyst for one-step vinyl chloride production from ethylene [CE-146]**  
Pedro A. Lira-Parada, ETH Zurich  
M. Scharfe, A.P. Amrute, J. Pérez-Ramírez

**One-pot conversion of aliphatic carboxylic acids to linear alpha olefins through tandem hydrogenation/dehydration [CE-147]**  
Jher Hau Yeap, EPF Lausanne  
B. Rozmysłowicz, J. Luterbacher

**Chirality transfer in prochiral substrates: proline-mediated asymmetric hydrogenation of isophorone on supported Pd catalyst [CE-148]**  
Fabian Meemken, ETH Zurich  
L. Rodriguez Garcia, K. Hungerbühler, A. Baiker

**Chemical Layer Deposition of metal oxide overcoats with targeted porosity by Stoichiometric and Kinetic control [CE-149]**  
Benjamin P. Le Monnier, EPF Lausanne  
F. Héroguel, J. Luterbacher

**Identification of the Active State of Platinum and the Role of Alkali Metal Promotion in Water-Gas Shift over Supported Pt Catalysts [CE-150]**  
Kanak Roy, ETH Zurich  
L. Artiglia, F. Orlando, A. Waldner, T. Huthwelker, J. A. van Bokhoven

**Mesoionic Iridium Complexes: Comparing CAN and Electrochemical Water Oxidation [CE-151]**  
Marta Olivares, University of Bern  
M. Li, C. Van der Ham, S. Bernhard, D. Hettterscheid, M. Albrecht

**Synthesis and Photocatalytic Water Oxidation Study of New Co<sub>4</sub>O<sub>4</sub> Cubane Complexes [CE-152]**  
Fangyuan Song, University of Zurich  
G. R. Patzke

**Circularly permuted and chimeric streptavidins as scaffolds for artificial metalloenzymes [CE-153]**  
Michela M. Pellizzoni, University of Basel  
C. Tinberg, D. Baker, F. Schwizer, T. R. Ward

**Activity Improvement by Immobilization and Protection of Artificial Imine Reductase on Silica Nanoparticles [CE-154]**  
Martina Ribar Hesticová, University of Basel  
R. Correro, M. Lenz, P. Shahgaldian, T. R. Ward

**Sol-Gel Processed Multicomposite Nanostructured Hematite-Titania Photoanode with Improved Oxygen Evolution: The Role of the Oxygen Evolution Catalyst [CE-155]**  
Mario Bärtsch, ETH Zurich  
R. Solaraska, M. Sarnowska, O. Krysiak, J. Augustyński, M. Niederberger

**Upregulation of an Artificial Zymogen by Proteolysis [CE-156]**  
Vincent Lebrun, University of Basel  
Z. Liu, T. Kitanosono, H. Mallin, V. Köhler, D. Häussinger, D. Hilvert, S. Kobayashi, T. R. Ward

**Unprecedented Activity of Silica-supported Tungsten-oxo in Olefin Metathesis [CE-157]**  
Ka Wing Chan, ETH Zurich

**V. Mougel, G. Siddiqui, K. Kawakita, H. Nagae, H. Tsurugi, O. V. Safonova, C. Copéret, K. Mashima**  
Selective deposition of zinc on copper surface by chemical vapor deposition, a selective catalyst for carbon dioxide-hydrogenation [CE-158]  
Saeed Saedy, Paul Scherrer Institute, Villigen  
J. Lee, M. Ranocchiari, J. A. van Bokhoven

**A Solvent Switchable Catalyst for the Transformation of HMF into Valuable Products [CE-159]**  
Sviatlana Siankevich, EPF Lausanne  
P. Dyson

**Isothermal stepped conversion of methane to methanol at elevated methane pressures [CE-160]**  
Marco Ranocchiari, Paul Scherrer Institute, Villigen  
P. Tomkins, J. A. van Bokhoven

**Earth abundant metal oxide nanoparticles as recyclable catalysts for N-methylation and N-formylation reactions using CO<sub>2</sub> as the C1 source in mild conditions [CE-161]**  
Aswin Gopakumar, EPF Lausanne  
P. J. Dyson

**Development of sulfur-tolerant ruthenium catalyst for dry biomass derived CO methanation [CE-162]**  
Dzulija Kuzmenko, Paul Scherrer Institute, Villigen  
M. Nachtgeal, T. Schildhauer, C. Copéret

### Inorganic Chemistry [IC] Poster Session

**Multitopic precursors for oxide materials' synthesis [IC-101]**  
Alba Finelli, University of Fribourg  
A. Crochet, K. Fromm

**Pressure induced chemisorption in isorecticular Metal Organic Frameworks [IC-102]**  
Piero Macchi, University of Bern  
A. Lanza, N. Casati, L. Germann, M. Fisch

**Controlling architecture of coordination cages *via* the aspect ratio of the ligands [IC-103]**

Suzanne Maria Jansze, EPF Lausanne  
K. Zhurov, M. Wise, R. Scopelliti, T. K. Ronson,  
J. R. Nitschke, K. Severin

**A Homoleptic Molybdenum(0) Complex with Chelating Isonitrile Ligands as a [Ru(bpy)<sub>3</sub>]<sup>2+</sup> Analog [IC-104]**

Laura Allegra Büldt, University of Basel  
O. S. Wenger

**Synergistic antimicrobial effect of silver and other metals in bimetallic complexes [IC-105]**

Paula C. Corcosa, University of Fribourg  
K. M. Fromm

**Thermodynamic and Photophysical Properties of Dual VIS/NIR Luminescent Erbium Complexes [IC-106]**

Bahman Golesorkhi, University of Geneva  
Y. Suffren, L. Guénée, H. Nozary, A. Hauser, C. Piguet

**Hydrolytic behaviour of mono- and dithiolato-bridged dinuclear arene ruthenium complexes and their interactions with biological ligands [IC-107]**

Julien Furrer, University of Bern  
L. Geiser, D. Stibal, G. Süss-Fink

**Screening of Dopants for Ceria-Based Materials for Solar Thermochemical Two-Step CO<sub>2</sub>-Splitting [IC-108]**

Roger Jacot, University of Zurich  
R. Michalsky, A. Steinfeld, G. R. Patzke

**Tuning the liquid-crystalline properties of pyrenyl-dendrimers by encapsulation in metallacycles [IC-109]**

Cristina Alvarino, University of Neuchâtel  
R. Deschenaux, B. Therrien

**Studies of Iridium Hydride Complexes and Recovery of Iridium Catalysts from Hydrogenation Reactions [IC-110]**

Stefan Gruber, University of Basel  
M. A. Müller, A. Pfaltz

**Development of new organometallic assemblies for photodynamic therapy applications [IC-111]**

Marie Gaschard, University of Neuchâtel  
B. Therrien

**Site-specific labeling of large RNA with fluorophores for the application in single molecule FRET studies [IC-112]**

Meng Zhao, University of Zurich  
F. Steffen, R. Börner, E. Freisinger, R. K. O. Sigel

***In situ* X-ray diffraction monitoring of the room temperature growth of Bi<sub>2</sub>O<sub>3</sub>CO<sub>3</sub> [IC-113]**

René Moré, University of Zurich  
M. Olah, Y. Zhou, G. R. Patzke

**New Light Emitting Electrochemical Cells with halogen containing [Cu(N<sup>^</sup>N)(P<sup>^</sup>P)][PF<sub>6</sub>] complexes [IC-114]**

Fabian Brunner, University of Basel  
S. Keller, A. Pertegás, H. J. Bolink, E. C. Constable,  
C. E. Housecroft

**Nitrous oxide as hydrogen acceptor for the dehydrogenative coupling of alcohols catalyzed by Rh(I) [IC-115]**

Thomas Gianetti, ETH Zurich  
S. P. Annen, G. Santiso-Quinones, M. Reiher,  
H. Grützmacher

**Hydrogen Bonded Arene Ruthenium Metalla-Assemblies [IC-116]**

Fan Zhang, University of Neuchâtel  
B. Therrien

**Highly active and stable iridium oxide and pyrochlore materials for oxygen evolution reaction [IC-117]**

Dmitry Lebedev, ETH Zurich  
D. Abbott, M. Povia, K. Waltar, E. Fabbri, A. Fedorov,  
T. Schmidt, C. Copéret

**Fighting Cancer with the Next Generation of Organometallic Assemblies [IC-118]**

Vidya Mannancherril, University of Neuchâtel  
B. Therrien

**Nucleophilic Reactivity of a Nitride-Bridged di-Uranium(IV) Complex: small molecules activation [IC-119]**

Marta Falcone, EPF Lausanne  
M. Mazzanti

**Heterometallic single precursor of oxides for Na-ion battery cathode materials [IC-120]**

Benoît Baichette, University of Fribourg  
K. M. Fromm

**Monodisperse Co-Sn, Fe-Sn, Co-Sb Alloy NCs as High Performance Li-Ion Battery Anodes [IC-121]**

Shutao Wang, ETH Zurich  
M. He, M. Walter, K. V. Kravchyk, F. Krumeich,  
M. V. Kovalenko

**Increasing kinetic inertness in polynuclear lanthanide complexes [IC-122]**

Davood Zare, University of Geneva  
Y. Suffren, L. Guénée, H. Nozary, S. V. Eliseeva, S. Petoud,  
A. Hauser, C. Piguet

**Improved spectral response does not lead to improved DSC performance: Studies on a ruthenium porphyrin-terpyridine conjugate [IC-123]**

Angelo Lanzilotto, University of Basel  
L. A. Büldt, H. Schmidt, A. Prescimone, O. S. Wenger,  
C. E. Housecroft, E. C. Constable

**Direct, aqueous carbon dioxide transformation to formic acid and methanol at room temperature [IC-124]**

Katerina Sordakis, EPF Lausanne  
G. Laurency

**Modifying spacers and anchoring groups for heteroleptic Cu(I)-6,6'-dimethyl-2,2'-bipyridine based DSSCs [IC-125]**

Maximilian Klein, University of Basel  
E. C. Constable, C. E. Housecroft

**Combining acid functionalized anchoring ligands with symmetric ancillary ligands in bis(diimine)copper(I) dyes in dye-sensitized solar cells – influence of the symmetry on the performance [IC-126]**

Annika Büttner, University of Basel  
E. C. Constable, C. E. Housecroft

**Chloro Ligand Enhancement of Water Oxidation Catalysis with a Pentapyridyl Ruthenium Complex [IC-127]**

Craig Richmond, University of Zurich  
C. Bachmann, D. Scherrer, L. Moser, T. Fox, B. Spingler,  
R. Alberto, C. Richmond

**Hierarchical graphene-based aerogels for long-life Li-ion batteries at high rates [IC-128]**

Guobo Zeng, ETH Zurich  
M. Niederberger

**Heteroleptic light-emitting copper(II) complexes with applications in light-emitting electrochemical cells (LECs) [IC-129]**

Sarah Keller, University of Basel  
C. E. Housecroft, A. Prescimone, E. C. Constable

**New Synthetic Strategies for  $[M(\eta^6\text{-arene})_2]^+$  ( $M = \text{Re}, {}^{99m}\text{Tc}$ ) Complexes [IC-130]**

Carla Gotzmann, University of Zurich  
H. Braband, R. Alberto

**Target Specific Multimodality Silica Nanoparticles for (Nano)Medical Applications [IC-131]**

Michel Wullemmin, University of Zurich  
H. Braband, R. Alberto

**Light-induced electron accumulation in a molecular triad [IC-132]**

Julia Nomrowski, University of Basel  
O. S. Wenger

**Silica nanoparticles functionalised with lanthanide luminescent complexes [IC-133]**

Atena B. Solea, Haute Ecole d'Ingénierie et d'Architecture Fribourg  
O. Mamula Steiner

**Photocatalytic hydrogen production using Co(II)-Complexes and Semiconductor Quantum Dots [IC-134]**

Fiorella Lucarini, University of Fribourg  
A. Ruggi

**Rhodium-Complexes for the Photochemical NAD(P)H Regeneration [IC-135]**

Mirjam Schreier, University of Basel  
M. Skaisgirski, O. S. Wenger

**Investigation of the interaction between platinum metal complexes and RNA G-quadruplex [IC-136]**

Zenghui Wang, University of Zurich  
A. Dominguez-Martin, S. Johannsen, R. Börner, Y. Zhong, Q. Cao, Z. Mao, R. K. O. Sigel

**Ring-modified Vitamin B<sub>12</sub> Derivatives as Potential Therapeutic Agents [IC-137]**

Lucas Prieto, University of Zurich  
R. Oetterli, B. Spingler, H. Brandl, M. Neuburger, F. Zelder

**Formic Acid Dehydrogenation Using Iron(II) Based Catalysts in Aqueous Media [IC-138]**

Mickael Montandon-Clerc, EPF Lausanne  
A. F. Dalebrook, G. Laurenczy

**Synthesizing Functionalized  $[M(\eta^6\text{-arene})_2]^+$  ( $\text{Re}, {}^{99m}\text{Tc}$ ) Complexes as Highly Stable Bioorganometallic Scaffolds for Receptor Targeting [IC-139]**

Giuseppe Meola, University of Zurich  
H. Braband, R. Alberto

**Hybrid lead and tin halide perovskites with guanidinium cation [IC-140]**

Olga Nazarenko, ETH Zurich  
M. Kotyrba, S. Yakunin, M. Wörle, M. V. Kovalenko

**Quantum Dots-sensitized Water Oxidation: Trick or Treat? [IC-141]**

Albert Ruggi, University of Fribourg

**N-Trifluoromethyl NHC Ligands Provide Selective Ruthenium Metathesis Catalysts [IC-142]**

Pascal Engl, ETH Zurich  
A. Fedorov, C. Copéret, A. Togni

**Investigating the benefits of incorporating carbohydrates into NHC systems for catalytic applications [IC-143]**

Joseph Peter Byrne, University of Bern  
M. Albrecht

**Chiral Iron(II) PNP Pincer Complexes for Enantioselective Direct Hydrogenation [IC-144]**

Raffael Huber, ETH Zurich  
A. Mezzetti

**Luminescence study of an anthracene derivative and its complexes with silver [IC-145]**

Noémie Voutier, University of Fribourg  
K. Fromm

**Synthesis and catalytic applications of chelating dicarbene iridium complexes [IC-146]**

Angela Vivancos, University of Bern  
M. Albrecht

**Highly Homo-perfluorinated Paramagnetic Ionic Liquids for NMR Field Probes for Magnetic Field Monitoring in MRI [IC-147]**

Anna C. Looser, University of Zurich  
S. Gross, C. Barmet, J. Nussbaum, R. Alberto, K. P. Prüssmann

**Reversible Quinone-based Relays as Electron Transporter in Artificial Photosynthesis [IC-148]**

Mathias Mosberger, University of Zurich  
C. Bachmann, B. Probst, R. Alberto

**Low Temperature Wet Conformal Nickel Silicide Formation on Silicon Wafer through an Organometallic Approach [IC-149]**

Tsung-Han Lin, ETH Zurich  
T. Margossian, M. d. Marchi, M. Thammasack, S. Kumar, C. Shih, D. Giovanni, D. Baudouin, P. Gaillardon, C. Copéret

**Energy efficient, low temperature hydrothermal synthesis of battery-grade LiFePO<sub>4</sub> platelet particles [IC-150]**

Peter Benedek, ETH Zurich  
M. Yarema, V. Wood

**Metal Oxide Catalysts for Alkane Functionalization [IC-151]**

Amanda Cook, ETH Zurich  
C. Copéret

**New routes to highly efficient copper(I)-based dye-sensitized solar cells: N<sup>4</sup>NX ligands as ancillary ligands [IC-152]**

Frederik J. Malzner, University of Basel  
E. C. Constable, C. E. Housecroft

**Controlling the Size of Nanocrystals of Metal-Organic Framework UiO-66 [IC-153]**

Marco Taddei, Paul Scherrer Institute, Villigen  
K. C. Dümbsgen, J. A. van Bokhoven, M. Ranocchiari

**Sn/C composite anode materials for high energy batteries [IC-154]**

Sivarajakumar Maharajan, University of Fribourg  
N. H. Kwon, K. M. Fromm

**Synthesis and characterization of novel imidazolium-based ionic-polystyrenes and their application as supports for Pd nanoparticles [IC-155]**

Felix D. Bobbink, EPF Lausanne  
A. Redondo, P. J. Dyson

**Highly Stable Red Light Emitting Electrochemical Cells Based on Cyclometallated Iridium(III) Complexes [IC-156]**

Cathrin D. Ertl, University of Basel  
C. Momblona, A. Pertegás, H. J. Bolink, E. Ortí,  
C. E. Housecroft, E. C. Constable

**A General Scheme for Oxidative Quenching of a Copper-bis-phenanthroline Photosensitizer for Light-Driven Hydrogen Production [IC-157]**

Johannes Windisch, University of Zurich  
M. Oraziotti, P. Hamm, B. Probst, R. Alberto

**Characterization and improvement of p-type dye sensitized solar cells [IC-158]**

Nathalie Marinakis, University of Basel  
C. E. Housecroft, E. C. Constable

**Evidence for [4+2] cycloaddition mechanism of alkynes to tantalacyclopentadiene as a model of alkyne cyclotrimerization [IC-160]**

Keishi Yamamoto, Osaka University  
H. Tsurugi, K. Mashima

**Isonitrile Iron(II) Complexes with Chiral (NH)<sub>2</sub>P<sub>2</sub> Macrocycles in the Enantioselective Transfer Hydrogenation of Polar Double Bonds [IC-161]**

Lorena De Luca, ETH Zurich  
R. Bigler, A. Mezzetti

**Cobalt(II)/Cobalt(III) Polypyridyl Complexes as Electrolytes in Combination with Copper(I) Dyes in Dye Sensitized Solar Cells [IC-162]**

Cedric Wobill, University of Basel  
S. Fürer, C. E. Housecroft, E. C. Constable

**Quasi-Solid Polymer Electrolytes reinforced by a Cellulose Nano Crystals to be used in Dye Sensitized Solar Cells [IC-163]**

Markus Willgert, University of Basel  
C. E. Housecroft, E. C. Constable

**Full magnetic investigations of a novel mononuclear 4f polyoxometalate exhibiting single molecule magnet behaviour [IC-164]**

Robin Güttinger, University of Zurich  
O. Blacque, A. Kostanyan, P.-E. Car, G. R. Patzke

**Synthesis and catalytic applications of O-functionalized mesoionic NHC metal complexes [IC-165]**

René Pretorius, University of Bern  
J. Olguín, M. Albrecht

**Strategies to solve the solution structure of the CPEB3 ribozyme through NMR spectroscopy [IC-166]**

Kenneth Adea, University of Zurich  
M. Skilandat, M. Rowinska-Zyrek, D. Donghi, S. Johannsen,  
R. K. O. Sigel

**New Perfluoroalkylated Reagents on the Basis of Hypervalent Iodine Compounds [IC-167]**

Mona Wagner, ETH Zurich  
N. Früh, M. Reiterer, A. Togni

**Growth of Zinc Oxide Rods on Wood Cross-sections to Fabricate Surfaces with Anisotropic Wettability [IC-168]**

Yaru Wang, ETH Zurich  
I. Burgert, E. Cabane

**Synthesis and reactivity of divalent lanthanide siloxide complexes [IC-169]**

Rory P. Kelly, EPF Lausanne  
M. Falcone, J. Andrez, R. Scopelliti, M. Mazzanti

**Facile post-modification to efficiently modulate the catalytic activity of triazolydene iridium complexes [IC-170]**

Karst Lenzen, University of Bern  
M. Albrecht

**A Cobalt-diketopyrphyrin complex as highly active catalyst for light-driven H<sub>2</sub> evolution [IC-171]**

Evelyne Joliat, University of Zurich  
N. Weder, C. Bachmann, B. Probst, B. Spingler, R. Alberto

**Synthesis of novel octadentate bifunctional chelating agents for <sup>89</sup>Zr immuno-PET [IC-172]**

Manon Briand, University of Zurich  
T. Mindt, G. Gasser

**Synthesis and catalytic activity of triazolydene iron(II) piano stool complexes [IC-173]**

Chloe Johnson, University of Bern  
M. Albrecht

**Direct Characterization of Highly Reactive Heterogeneous Alkene Metathesis Catalyst by DNP SENS [IC-174]**

Wei-Chih Liao, ETH Zurich  
T. Ong, D. Gajan, G. Casano, M. Pucino, O. Ouari,  
A. Lesage, P. Tordo, L. D. Emsley, C. Copéret

**Heterometallic coordination cages with unusual geometries [IC-175]**

Giacomo Cecot, EPF Lausanne

**Molecular Knots and Links for Halide Binding and Allosterically Regulated Catalysis [IC-176]**

Alexander Stephens, University of Basel  
A. L. Nussbaumer, S. L. Woltering, R. G. Pritchard,  
J. J. Danon, J. Lemonnier, D. A. Leigh

**New Polarization Matrices for Dynamic Nuclear Polarization with the Polarizing Agent Embedded in the Wall [IC-177]**

Daniel L Silverio, ETH Zurich  
H. A. van Kalker, T. Ong, M. Yulikov, D. Gajan,  
G. Jeschke, M. V. Kovalenko, C. Thieuleux, C. Copéret,  
L. Emsley

**Formation of Formic Acid via CO<sub>2</sub> Hydrogenation with Silica-Supported Transition Metal Pincer Complexes [IC-178]**

Hung-Kun Lo, ETH Zurich  
I. Thiel, C. Copéret

**Molecular photocathodes for hydrogen evolution [IC-179]**

Nicolas Kaeffer, ETH Zurich  
J. Massin, V. Artero

**Propane Dehydrogenation Utilizing Gallium-Based Catalysts [IC-180]**

Keith Searles, ETH Zurich  
G. Siddiqui, K. Bodmer, C. Copéret

**Bis-Pyridylidene Amide Ligands for Ruthenium-Facilitated Oxidation Processes [IC-181]**

Kevin Salzmann, University of Bern  
C. Segarra, M. Albrecht

**Donor-Adaptive N-Mesoionic Ligands for Ruthenium-Mediated Redox Catalysis [IC-182]**

Candela Segarra, University of Bern  
N. Meisel, K. Salzmann, M. Albrecht

**Oriented crystallization of barite in hierarchical cell structures [IC-183]**

Vivian Marina Merk, ETH Zurich  
J. K. Berg, C. Krywka, I. Burgert

**A naked-eye [Ce<sub>2</sub>(HXTA)]<sup>3+</sup> based biosensor for the detection of phosphate ions in water [IC-184]**

Thibaud Rossel, Gymnase français de Bienne/University of Bern  
M. Creus

**Medicinal Chemistry & Chemical Biology [MC]  
Poster Session****Bacterial Resistance to Silver: The Role of SilE Protein [MC-101]**

Valentin Chabert, University of Fribourg  
K. M. Fromm

**The discovery of a potent and orally available Dot1L inhibitor [MC-103]**

Christian Ragot, Novartis Pharma AG  
C. Mura, F. Stauffer

**Oligoprolines as Scaffolds for Tumor Targeting with Hybrid Bombesin Analogues [MC-104]**

Stefanie Dobitz, ETH Zurich  
C. Kroll, R. Mansi, F. Braun, H. Mäcke, H. Wennemers

**Potency is not enough. SwissADME: a web tool to support medicinal chemists in the pharmacokinetic optimization of small molecules [MC-105]**

Antoine Daina, SIB Swiss Institute of Bioinformatics, Molecular Modeling Group  
O. Michielin, V. Zoete

**Microwave assisted synthesis of the antimicrobial peptide dendrimer G3KL [MC-106]**

Thisa N. Siriwardena, University of Bern  
M. Heitz, T. Darbre, J.-L. Reymond

**Development of specific probes for the visualization of bivalent epigenetic marks in live cells [MC-107]**

Aurore Delachat, EPF Lausanne  
O. Pundel, N. Guidotti, H. Pick, B. Fierz

**Eudesmane sesquiterpenes from *Verbesina lanata* with inhibitory activity against major agricultural pathogens [MC-108]**

Justine Ramseyer, University of Basel  
B. Thuerig, M. De Mieri, H. Schäfer, L. Tamm, O. Potterat, M. Hamburger

**Development of Synthesis Methodology for DNA-encoded Chemical Libraries [MC-109]**

Andreas Brunschweiler, Technische Universität Dortmund

**Molecular interactions in crystal packing of dipeptide gels [MC-110]**

Anja Holzheu, University of Fribourg  
A. Crochet, A. Apicella, K. Fromm

**In vivo Assay for Artificial Metalloenzyme Evolution [MC-111]**

Fabian Schwizer, University of Basel  
T. Heinisch, T. R. Ward

**Orally Bioavailable Antimalarial 4(1H)-Quinolone Prodrugs with Single-Dose Cures [MC-112]**

Fabian Brockmeyer, Northeastern University Boston  
A. Monastyrskiy, A. LaCrue, T. Mutka, D. Kyle, R. Manetsch

**De novo drug design revisited [MC-113]**

Gisbert Schneider, ETH Zurich

**Gut microbes and probiotics anaerobically transform carcinogenic dietary heterocyclic amines to metabolites with altered toxicity [MC-114]**

Jianbo Zhang, ETH Zurich  
C. Engels, M. Schneider, M. Fekry, C. Lacroix, S. Sturla

**Assignment of absolute configuration in labdane and clerodane diterpenoids [MC-115]**

Maria De Mieri, University of Basel  
K. Du, M. Neuburger, D. Ferreira, M. Hamburger

**EgtB from Ergothioneine Biosynthesis – Mechanistic and Evolutionary Insights using Protein Crystallography [MC-116]**

Anja Stampfli, University of Basel  
F. Seebeck

**Labelling strategies for studying the folding and splicing of the wild type group II intron ai5g [MC-117]**

Maya Gulotti-Georgieva, University of Zurich  
M. Zhao, F. Steffen, R. K. O. Sigel

**Extending carbocyanine photophysics to the realm of RNA [MC-118]**

Fabio Steffen, University of Zurich  
R. K. O. Sigel, R. Börner

**RNA G-quadruplex formation within the BCL2 human oncogene: towards its structural determination [MC-119]**

Alicia Dominguez-Martin, University of Zurich  
R. K. O. Sigel

**Functionalization of second harmonic generation nanoparticles for theranostic applications [MC-120]**

Jérémy Vuilleumier, EPF Lausanne  
R. De Matos, S. Passemard, L. Bonacina, S. Gerber

**Investigation of the interaction between 5-HT<sub>3</sub>R and its modulators: progress in understanding the agonist binding site [MC-121]**

Martin Lochner, University of Bern  
T. Jack, J. Simonin, M. Leuenberger, P. Rüefli, Y. Bur, C. Hechavarría, M.-D. Ruepp, A. J. Thompson

**Peptide dendrimer as siRNA transfection reagent [MC-122]**

Marc Heitz, University of Bern  
T. Darbre, J.-L. Reymond

**New insights into glutamate transport in brain: Concise asymmetric synthesis of TFB-TBOA and photoaffinity probes [MC-123]**

Michele Leuenberger, University of Bern  
A. Ritler, V. Aerni, S. G. Metzger, M.-D. Ruepp, M. Lochner

**Polyoxometalate-chitosan nanocomposites for medical applications [MC-124]**

Matteo Croce, University of Zurich  
S. Conti, C. Maake, G. R. Patzke

**Design, synthesis and pharmacological characterization of novel store-operated calcium channel (SOCE) modulators [MC-125]**

Achille Schild, University of Bern  
D. Tscherrig, N. Wenger, B. Rajesh, B. Lüscher, M. A. Hediger, M. Lochner

**Total Synthesis, Target Evaluation and Structure-Activity Studies of Mycolactone and its Analogs [MC-126]**

Matthias Gehring, ETH Zurich  
P. Gersbach, R. Bieri, N. Scherr, G. Pluschke, K.-H. Altmann

**Functionalization of second harmonic nanoparticles for targeted tumor imaging and multimodal cancer diagnosis [MC-127]**

Raphaël De Matos, EPF Lausanne  
S. Passemard, D. Staedler, S. Constant, L. Bonacina,  
S. Gerber

**Discovery of TRPM4 ion channel inhibitors [MC-128]**

Clémence Delalande, University of Berne  
L. Ozhatil, B. Bianchi, H. Abriel, J.-L. Reymond

**Identification and improvement of modulators of Divalent Metal Ion Transporter 1 (DMT1) [MC-129]**

Marion Poirier, University of Bern  
A. Embaby, J. Pujol-Giménez, M. A. Hediger,  
J.-L. Reymond

**Functionalized Proline-Rich Peptides as Selective Binders of c-diGMP [MC-130]**

Carlotta Foletti, ETH Zurich  
R. A. Kramer, K. H. Bleicher, J. Kisunzu, H. Wennemers

**Substitutions of Methionine on DOTA-Minigastrin 11: Evaluation of two non-natural amino acids [MC-131]**

Nathalie Grob, ETH Zurich  
M. Béhé, R. Schibli, T. Mindt, T. L. Mindt

**A close look to the interaction of a metallo-intercalator and an RNA internal loop via NMR [MC-132]**

Elena Alberti, University of Zurich  
M. Coogan, D. Donghi

**Metal ion interactions in ncRNAs revealed by smFRET [MC-133]**

Richard Börner, University of Zurich  
R. K. O. Sigel

**HPLC-based activity profiling for GABA<sub>A</sub> receptor modulators from *Searsia pyroides* leaves using a validated larval zebrafish locomotor assay [MC-134]**

Fahimeh Moradi-Afrapoli, University of Basel  
S. N. Ebrahimi, H. van der Merwe, M. Smiesko,  
M. Hamburger

**Click Chemistry for DNA Interstrand Crosslinking [MC-135]**

Zahra Harati-Taji, University of Zurich  
N. W. Luedtke

**Pre-organization of Selectin Antagonist: Novel Structural Modifications [MC-136]**

Norbert Varga, University of Basel  
P. Zihlmann, T. Mühlethaler, M. Smiesko, B. Ernst

**Target-Driven Dynamic Combinatorial Chemistry – Potentials and Pitfalls as Exemplified on a Bacterial Adhesin [MC-137]**

Priska Frei, University of Basel  
L. Pang, D. Eris, M. Silbermann, T. Mühlethaler,  
O. Schwardt, B. Ernst

**Inhibition of SHMT: A Neglected Enzyme from the Folate Cycle [MC-139]**

Geoffrey Schwertz, ETH Zurich  
M. Witschel, M. Rottmann, R. Bonnert, P. Chaiyen,  
P. Chitnumsub, K. White, F. Diederich

**The Moco Ribswitch from E. Coli [MC-140]**

Fabio Amadei, University of Zurich  
S. Gallo, R. Börner, R. K. O. Sigel

**The Influence of the Ester Prodrug Hydrolysis upon Bioavailability of FimH Antagonists [MC-141]**

Philipp Dätwyler, University of Basel  
J. Bezençon, A. Sigl, S. Kleeb, W. Schönemann, B. Ernst

**Berberine dimer as a turn-on fluorescent G-quadruplex ligand by its conformational switching [MC-142]**

Masayuki Tera, University of Zurich  
T. Hirokawa, K. Sugahara

**Radiosynthesis of Eight Radiotracers via Cu-mediated <sup>18</sup>F-Fluorination of Aryl Boronic Esters on a Clinically Relevant Scale [MC-143]**

Sean Preshlock, University of Oxford  
S. Calderwood, S. Verhoog, M. Tredwell, S. Gruber,  
T. C. Wilson, N. J. Taylor, M. Huiban, V. Gouverneur

**Fluorescent Labeling of the Antimicrobial Peptide Dendrimer G3KL to Investigate its Mechanism of Action against *Pseudomonas aeruginosa* [MC-144]**

Bee Ha Ha Gan, University of Bern  
T. Darbre, J.-L. Reymond

**Impact of pathogen inactivation technologies on platelets: cell functionality and redox proteome [MC-145]**

Giona Sonogo, Transfusion InterRégionale  
M. Prudent, M. Abonnenc, D. Crettaz, J. Tissot, N. Lion

**Probing the cellular uptake and response of porphyrinic photosensitizers in polymeric nanoparticles by fluorescence measurements and <sup>1</sup>H HR-MAS NMR based metabolic profiling of HeLa cells [MC-147]**

Sara Pfister, University of Bern  
I. Gjuroski, D. Nydegger, M. Hädener, G. Diserens,  
P. Vermathen, J. Furrer, M. Vermathen

**Polymer Delivery Systems of Porphyrin Photosensitizers Monitored by NMR Spectroscopy [MC-148]**

Ilche Gjuroski, University of Bern  
S. Pfister, J. Furrer, M. Vermathen

**Efficacy of Block Copolymers to Disaggregate and Encapsulate Porphyrins Monitored by NMR Spectroscopy [MC-149]**

Ilche Gjuroski, University of Bern  
S. Pfister, J. Furrer, M. Vermathen

**Can Nanoparticle Carrier Systems decrease the Reactivity of Porphyrinic Photosensitizers towards Serum and Cytosolic Proteins? [MC-150]**

Martina Vermathen, University of Bern  
L. Sauser, I. Gjuroski, J. Furrer

**Rapid-Acting Insulin Analog Engineering using Multipolar Force Fields: Stabilization of a Protein Crevice by Halo-Aromatic Substitutions [MC-151]**

Krystal El Hage, University of Basel  
M. A. Weiss, M. Meuwly

**Spectroscopic and structural studies of histidine-rich metallothioneins [MC-152]**

Jelena Habjanic, University of Zurich  
O. Zerbe, E. Freisinger

**Further insights into the cadmium specificity of Necln\_MT1 [MC-153]**

Monica Perinelli, University of Zurich

**Synthesis and Biological Activity of New SLC7A5/LAT1 Inhibitors [MC-154]**

Julien Graff, ETH Zurich  
J. Gertsch, K.-H. Altmann

**Active metal-based drugs delivery using vitamin B<sub>12</sub> as a carrier [MC-155]**  
 Rossier Jérémie, University of Fribourg  
 F. Zobi

**Exploitation of the allosteric relationship between RAPTA-T and Auranofin on the Nucleosome Core Particle in the design of novel anti-cancer agents [MC-156]**  
 Lucinda Batchelor, EPF Lausanne  
 E. Paunescu, G. Palermo, U. Röthlisberger, C. A. Davey, P. Dyson

**Endogenous Formation of N-Nitroso Compounds by Gut Microbiota [MC-157]**  
 Simon Sieber, ETH Zurich  
 C. Lacroix, S. Sturla

**A thioether ligated cyclic antimicrobial undecapeptide with D,L-architecture targeting multidrug resistant *Pseudomonas aeruginosa* [MC-158]**  
 Ivan Di Bonaventura, University of Bern  
 R. He, J.-L. Reymond

**Studying histone ubiquitination on chemically defined chromatin [MC-159]**  
 Andreas L. Bachmann, EPF Lausanne  
 L. Bryan, B. Fierz

**The role of substrate hydrogen bonding in the non-heme iron enzyme EgtB [MC-160]**  
 Reto Burn, University of Basel  
 K. Goncharenko, F. Seebeck

**Design and synthesis of highly potent and upmost selective acetylbenzenes as CREBBP ligands [MC-161]**  
 Aymeric Dolbois, University of Zurich  
 A. Unzue, A. Caflisch, C. Nevado

**Fluorescent Flippers on a Monolayer [MC-162]**  
 Frederik Neuhaus, University of Fribourg  
 A. Zumbühl, S. Matile

**Following the splicing process of an encapsulated group II intron by single-molecule FRET [MC-163]**  
 Besim Fazliji, University of Zurich  
 S. Zelger-Paulus, M. C. Hadzic, R. Börner, R. K. O. Sigel

**Palladium nanoparticles for the specific modification of native proteins [MC-164]**  
 Anaëlle Dumas, Université Paris-Sud  
 A. Peramo, D. Desmaële, P. Couvreur

**Polarizing solids (HYPSO) for DNP applications [MC-165]**  
 Matthieu Cavaillès, CPE Lyon  
 D. Baudouin, A. Bornet, S. Jannin, A. Lesage, G. Bodenhausen, L. Emsley, C. Copéret, C. Thieuleux

**Antimicrobial Activity and Stability of Diastereomeric Peptide Dendrimers [MC-166]**  
 Stéphane Baeriswyl, University of Bern  
 T. N. Siriwardena, T. Darbre, J.-L. Reymond

**Fluorescent modified DNA to detect frameshift mutation [MC-167]**  
 Florence D. Berger, ETH Zurich  
 S. Sturla, R. Manderville

**Platinum-Porphyrin Conjugates in Photodynamic Therapy [MC-168]**  
 Michele Larocca, University of Zurich  
 B. Spingler

**SwissDrugDesign [MC-169]**  
 Vincent Zoete, SIB Swiss Institute of Bioinformatics  
 A. Daina, D. Haake, C. Bovigny, O. Michielin

**A new Epitope Mimetic of the MPER in HIV-1 gp41 [MC-170]**  
 Mylène Morin, University of Zurich  
 E. Stiegeler, N. Friedrich, T. Reinberg, K. Moehle, S. Hansen, A. Marrero Nodarse, A. Trkola, A. Plückthun, J. A. Robinson

**Modifying Phenotypes by Chemical Cell Surface Engineering [MC-171]**  
 Isabel P. Kerschgens, University of Zurich  
 K. Gademann

### Organic Chemistry [OC] Poster Session

**Decoding the Biological Mechanisms of Buruli Ulcer Thanks to a modular Total Synthesis [OC-102]**  
 Sarah Saint-Auret, CNRS - Université de Strasbourg  
 P. Bisseret, N. Blanchard

**Photoresponsive self-healing supramolecular hydrogels for light-induced release of bioactive guests [OC-103]**  
 Zbigniew Pianowski, Karlsruher Institut für Technologie (KIT)  
 J. Karcher, K. Schneider

**Paramagnetic Photoredox-Switchable Molecular Grippers: The Elements of Six-State Redox Switches [OC-104]**  
 Jovana Milic, ETH Zurich  
 M. Zalibera, I. Pochorowski, J. Nomrowski, D. Neshchadin, L. Ruhlmann, C. Boudon, O. S. Wenger, G. Gescheidt, W. Lubitz, F. Diederich

**Cell-Penetrating Poly(disulfide)s [OC-105]**  
 Paola Morelli, University of Geneva  
 G. Gasparini, N. Chuard, E. Bartolami, A. Roux, N. Sakai, S. Matile

**The Third Orthogonal Organic Dynamic Covalent Bond [OC-106]**  
 Santiago Lascano, University of Geneva  
 K. Zhang, R. Wehlauch, K. Gademann, N. Sakai, S. Matile

**Stereoselective Metal-Free Synthesis of  $\beta$ -Amino Thioesters and their Synthetic Application [OC-107]**  
 Oliver Engl, ETH Zurich  
 E. Cosimi, M.-O. Ebert, J. Saadi, H. Wennemers

**Palladium(0)-Catalyzed Asymmetric C(sp<sup>3</sup>)-H Arylation: the Chiral Base Approach [OC-108]**  
 Lei Yang, University of Basel  
 R. Melot, O. Baudoin

**Towards the Total Synthesis of Lathyrane A [OC-109]**  
 Giulia Rusconi, University of Zurich  
 M. Arthuis, A. Lorente, C. Nevado

**Rh(III)-catalyzed asymmetric synthesis of *P*-stereogenic heterocycles from phosphamides [OC-110]**  
 Yang Sun, EPF Lausanne  
 N. Cramer

**Stereoselective Organocatalyzed Synthesis of  $\beta$ -Amino Thioesters and  $\gamma$ -Nitro Thioesters and Their Synthetic Application [OC-111]**

Elena Cosimi, ETH Zurich  
O. Engl, H. Wennemers

**Modular electrophilic tetrafluoroalkylation reagents tailored for selective and irreversible thiol bioconjugation [OC-112]**

Jiri Vaclavik, ETH Zurich  
V. Matoušek, I. Klimánková, P. Beier, A. Togni

**Aqueous Titanium Trichloride-Promoted Reductive Cyclization of *o*-Nitrostyrenes to Indoles [OC-113]**

Mathias Mamboury, EPF Lausanne  
S. Tong, Z. Xu, Q. Wang, J. Zhu

**Fast and Highly Chemoselective Alkynylation of Thiols with Hypervalent Iodine Reagents [OC-114]**

Romain Tessier, EPF Lausanne  
D. Hari, R. Frei, J. Waser

**Pd(0)-Catalyzed Enantioselective Synthesis  $\alpha$ -Alkynyl, Azido and Cyano Ketones [OC-115]**

Paola Caramenti, EPF Lausanne  
M. V. Vita, J. Waser

**New Approach Towards Nucleophilic Tetrafluoroethylation [OC-116]**

Alena Budinská, Academy of Sciences of the Czech Republic  
J. Vaclavik, V. Matoušek, A. Togni, P. Beier

**Efforts toward the Total Synthesis of Hyperforin via a Tandem Strategy [OC-117]**

Richard Remy, University of Fribourg  
C. Bochet

**Lipid Linked Oligosaccharide (LLO) Analogues as Oligosaccharyltransferase (OST) Substrates [OC-118]**

Jérémy Boilevin, University of Bern  
K. Locher, T. Darbre, J.-L. Reymond

**A green one-pot synthesis of a magnetic mesoporous carbon-containing Pd-Co nanoalloy. Applications for Suzuki couplings [OC-119]**

Claude Le Drian, Université de Haute-Alsace, Mulhouse, France  
C. Matei-Ghimbeu, J.-M. Becht

**Stereoselective Arene-Forming Aldol Condensation: Synthesis of Axially Chiral Aromatic Amides [OC-120]**

Vincent Fäseke, University of Basel  
C. Sparr

**Highly  $\gamma$ -selective allylation of (*E*)-alkenylzinc iodides prepared by reductive coupling of arylacetylenes with alkyl iodides [OC-121]**

Fedor Zhurkin, EPF Lausanne  
X. Hu

**Peptide-Catalyzed Stereoselective Conjugate Addition Reactions of Aldehydes to Maleimides [OC-122]**

Claudio Grünenfelder, ETH Zurich  
J. Kisunzu, H. Wennemers

**Volcano Plots: Computational Tools for Screening Homogeneous Catalysts [OC-123]**

Matthew Wodrich, EPF Lausanne  
M. Busch, C. Corminboeuf

***N*-Heterocycles via Pd(0)-Catalysed C(sp<sup>3</sup>)-H Functionalisation [OC-124]**

Julia Pedroni, EPF Lausanne  
N. Cramer

**Synthesis of a Tetracyclic Derivative of Norbornane [OC-125]**

Lorenzo Delarue Bizzini, University of Basel  
M. Mayor

**[4+2]-Annulations of Aminocyclobutanes [OC-126]**

Daniele Perrotta, EPF Lausanne  
S. Racine, F. de Nanteuil, J. Waser

**Room-Temperature Decarboxylative Alkynylation of Carboxylic Acids Using Photoredox Catalysis and EBX Reagents [OC-127]**

Franck Le Vaillant, EPF Lausanne  
T. Courant, M. Wodrich, J. Waser

**Alleno-Acetylenic Cages (AACs): Conformational Chirality Switch and Molecular Recognition [OC-128]**

Cornelius Gropp, ETH Zurich  
N. Trapp, F. Diederich

**Conformational Analysis of Tripeptide Catalysts Using Computational Methods and NMR Spectroscopy [OC-129]**

Jessica Kisunzu, ETH Zurich  
C. Rigling, M.-O. Ebert, H. Wennemers

**Palladium-Catalyzed Enantioselective Intermolecular Carboetherification of Dihydrofurans [OC-130]**

Gustavo M. Borrajo-Calleja, University of Geneva  
V. Bizet, C. Mazet

**Asymmetric Morita-Baylis-Hillman Reaction: Catalyst Development and Mechanistic Insights [OC-131]**

Patrick Isenegger, University of Basel  
A. Pfaltz

**Lewis Acid-Catalyzed  $\alpha$ -Perfluoroalkylation of Ketene Silyl Acetals and Ketene Silyl Amides [OC-132]**

Dmitry Katayev, ETH Zurich  
V. Matousek, J. Vaclavik, A. Togni

**Palladium-Catalyzed Long-Range Deconjugative Isomerization of Highly Substituted  $\alpha,\beta$ -Unsaturated Carbonyl [OC-133]**

Ciro Romano, University of Geneva  
L. Lin, C. Mazet

**Radical Chemistry of Gem-Diboronates [OC-134]**

Andrey Kuzovlev, University of Bern  
M. Lüthy, P. Renaud

**Radical-Mediated Enantioselective Hydroazidation of Alkenes [OC-135]**

Daniel Meyer, University of Bern  
P. Renaud

**Simplified strigolactams as potent analogues of strigolactones for the seed germination induction of *Orobancha cumana* Wallr [OC-136]**

Alexandre Lumbroso, Syngenta Crop Protection AG  
E. Villedieu-Percheron, D. Zurwerra, C. Screpanti, M. Lachia, P.-Y. Dakas, L. Castelli, V. Paul, R. Fonne-Pfister, A. de Mesmaeker

**Preparation of Alkylated Pyridine Derivatives via Radical Addition to *N*-Methoxypyridinium Salts [OC-137]**

Samuel Rieder, University of Bern  
I. Gorokhovic, P. Renaud

**Photo Chemical Amplifier Based Self-Immolative Spacer**

[OC-138]

Agonist Kastrati, University of Fribourg  
C. Bochet**Trialkylation of cyclic thioiminium ions [OC-139]**Melinda Mojzesova, University of Bern  
P. Mateo, P. Renaud**New access to quaternary aminocyclobutanes via nucleophilic additions on cyclobutaniminium salts [OC-140]**Amandine Kolleth-Krieger, Syngenta Crop Protection AG  
A. Lumbroso, G. Tanriver, S. Catak, S. Sulzer,  
A. de Mesmaeker**Template-free high hierarchical self-assembly of a pyrene derivative into supramolecular nanorods [OC-141]**Mohamed El Idrissi, University of Applied Sciences and Arts  
Northwestern Switzerland, FHNW  
P. Shahgaldian**Exploring Site Selectivity of Iridium Hydride Insertion into Allylic Alcohols: Serendipitous Discovery of a Mild and General Catalyst for the Vinylogous Peterson Elimination [OC-142]**Daniele Fiorito, University of Geneva  
H. Li, C. Mazet**Terminal-selective arylation of alkyl chains by regio-convergent Negishi coupling [OC-143]**Ke-Feng Zhang, University of Basel  
S. Dupuy, A. Goutierre, O. Baudoin**Synthesis of amino-cyclobutanes via [2+2] cycloadditions involving keteniminium intermediates [OC-144]**Amandine Kolleth-Krieger, Syngenta Crop Protection  
A. Lumbroso, G. Tanriver, S. Catak, S. Sulzer,  
A. de Mesmaeker**Anion- $\pi$  Interactions and Chalcogen Bonding in Functional Systems [OC-145]**Sebastian Benz, University of Geneva  
Y. Cotelte, M. Maccione, L. Liu, N. Sakai, S. Matile**Atom Economical Transformation of Ethynyl-benziodoxol(on)e (EBX) Reagents: Oxy-Alkynylation of Diazo Compounds [OC-146]**Durga P. R. Hari, EPF Lausanne  
J. Waser**Pd(0)-Catalyzed Enantioselective C-H Functionalization of Enamide Phosphates [OC-147]**Daria Grosheva, EPF Lausanne  
N. Cramer**Carbohydrate mimics for therapeutic applications: exploring their conformational preference in the gas and micro-hydrated phases [OC-148]**Maja Kandziora, University of Basel  
O. Schwardt, P. Çarçal, M. Smiesko**Toward a Computationally Holistic View of Homogeneous Catalysis [OC-149]**Michael Busch, EPF Lausanne  
M. Wodrich, C. Corminboeuf**Ruthenium-Catalyzed [2+2] Cycloaddition Reactions of Bicyclic Alkenes with 1-Alkynyltriazenes [OC-150]**Florian G. Perrin, EPF Lausanne  
A. A. Suleymanov, K. Severin**Enantioselective  $\alpha$ -arylation of protected aliphatic alcohols via sparteine-mediated asymmetric lithiation and Negishi coupling [OC-151]**Titouan Royal, University of Basel  
Y. Baumgartner**Study of Gold(III)-fluoride complexes: Key Intermediates in Gold Catalyzed Transformations [OC-152]**Roopender Kumar, University of Zurich  
A. Linden, C. Nevado**N-formylation of Amines with CO<sub>2</sub> Catalyzed by Fluoride and Hydroxide Anions [OC-153]**Martin Hulla, EPF Lausanne  
F. D. Bobbink, S. Das, P. Dyson**Towards the Total Synthesis of Leiodolide A [OC-154]**Adriana Edenharter, ETH Zurich  
K.-H. Altmann**The Mechanism of Stereospecific Cyclization: Key Step on the Way to Optically Active Chromans [OC-155]**Thomas Netscher, DSM Nutritional Products  
A. Loesche**Oligoprolines as a Versatile Platform for the Self-Assembly of  $\pi$ -Systems [OC-156]**Urszula Lewandowska, ETH Zurich  
W. Zajackowski, W. Pisula, S. Corrà, N. Ochs, S. Steppert,  
C. Li, K. Müllen, H. Wennemers**Tailor-made Concave Ligands for the Encapsulation and Functionalization of Nanoparticles [OC-157]**Almudena Gallego, University of Basel  
M. Mayor**Organocatalytic enantioselective Michael addition of  $\alpha$ -alkyl substituted  $\alpha$ -nitroacetates to phenyl vinyl selenone [OC-158]**Antonin Clemenceau, EPF Lausanne  
J. Zhu, Q. Wang**Helical oligophenyl Geländer molecules [OC-159]**Rajesh Mannancherry, University of Basel  
M. Mayor**Multifold-Linked Fe(II) Terpyridine Cage Complexes [OC-160]**Thomas Brandl, University of Basel  
M. Mayor**Studying the conformational ensemble of b<sup>3</sup>/b<sup>2</sup>-peptides using ROEs, J-couplings and RDCs [OC-161]**Carla Rigling, ETH Zurich  
B. Kolesinka, M.-O. Ebert**Thiol-Catalyzed Radical Deuteration of Alkyl Iodides Mediated by Triethylborane and Deuterium Oxide [OC-162]**Valentin Soulard, University of Bern  
G. Villa, D. Vollmar, P. Renaud**EthynylBenziodoxolone (EBX) Reagents for Alkynylation Reactions [OC-163]**Lionel Schouwey, EPF Lausanne  
J. Waser**Organocatalyzed 1,4-addition reactions of aldehydes to nitroolefins – Mechanistic studies [OC-164]**Patrick Hilpert, ETH Zurich  
H. Wennemers

**Chiral Cp<sup>X</sup>Ir(III) Catalyzed C-H Amidation Leading to P-Chiral Arylphosphine Oxides [OC-165]**

Yun-Suk Jang, EPF Lausanne  
M. C. Dieckmann, N. Cramer

**Retention of Absolute Configuration in Hydrogen Atom Transfer/Cyclisation Cascade [OC-166]**

Christian Gloor, University of Bern  
I. Kovalova, V. Soulard, P. Locher, Y. Kavanagh,  
M. Pichowicz, P. Renaud

**Neutral Radicals Derived From Imidazolium Dyes [OC-167]**

Léonard Yannick Maurice Eymann, EPF Lausanne  
A. Tskhovrebov, M. Wodrich, L. Vannay, C. Corminboeuf,  
K. Severin

**Catechol Mediated Intermolecular Carbohydrogenation of Terminal and Non-Terminal Alkenes [OC-168]**

Sankar Rao Suravarapu, University of Bern  
S. Rieder, G. Povie, P. Renaud

**Synthesis of Persistent Derivative of Open Shell Graphene Fragment Triangulene [OC-169]**

Peter Ribar, University of Basel  
M. Juricek

**Development of fluorescent nucleoside isosteres [OC-170]**

Aaron Johnson, University of Zurich  
N. W. Luedtke

**Spin-Delocalized Hydrocarbons With or Without Twist [OC-171]**

Michal Juricek, University of Basel  
P. Ravat, P. Ribar, T. Solomek

**Studies on the alkene-tetrazine ligation for DNA labeling [OC-172]**

Anna Bujalska, University of Zurich  
N. W. Luedtke

**Sulfonyl Radical Mediated Addition/Translocation/Cyclization Cascade [OC-173]**

Christian Gloor, University of Bern  
F. Dénès, P. Renaud

**Supramolecular architectures based on a novel AAA-DDD triple hydrogen bonding motif [OC-174]**

Jonathan Y. Grolms, EPF Lausanne  
K. Severin

**Intermolecular H-Atom Abstraction in Radical C-H Activation [OC-175]**

Ievgeniia Kovalova, University of Bern  
P. Renaud

**Catalyst-Controlled Diastereoselective Isomerization of Acyclic Primary Allylic Alcohols [OC-176]**

Julien Guillemin, University of Geneva  
H. Li, C. Mazet

**High resolution F1-decoupled NMR spectra for the analysis of mixture of compounds with similar structure [OC-177]**

Marta Brucka, University of Geneva  
D. Jeannerat

**Atomistic simulations of Claisen rearrangement reaction in solution and enzyme environment [OC-178]**

Sebastian Brickel, University of Basel  
M. Meuwly

**Gold-Catalyzed Alkynylation of Arenes: Mechanistic Insights and Evidence for Au<sup>I</sup>/Au<sup>III</sup> Redox Catalytic Cycles [OC-179]**

Manuel Hofer, University of Zurich  
T. De Haro, E. Gomez-Bengoia, R. Kumar, C. Nevado

**Synthesis towards a new Diacetylene Bridged Geländer-Type Oligomer [OC-180]**

Linda M. Bannwart, University of Basel  
M. Mayor

**Gold Nanoparticles Reaching out for Molecular Electronics via Tailor-Made Ligands [OC-181]**

Erich H. Peters, University of Basel  
M. Lehmann, M. Mayor

**Synthetic Low Density Lipoprotein with Surface Functionalization [OC-182]**

Sean Oriana, ETH Zurich  
Y. Yamakoshi

**Synthesis and characterization of novel cross-linked ionic polymers and their application for carbon dioxide cycloaddition to epoxides [OC-183]**

Antoine van Muyden, EPF Lausanne  
F. D. Bobbink, P. J. Dyson

**Physical Chemistry [PC]  
Poster Session****Structure-Activity Relationship of Photoinitiators for Two Photon Polymerisation [PC-101]**

Joseph S. Beckwith, University of Geneva  
A. Rosspeintner, G. Licari, M. Lunzer, J. Fröhlich,  
E. Vauthey

**Fast and accurate prediction of covalent bonds in chemical space [PC-102]**

K. Y. S. Chang, University of Basel  
S. Fias, R. Ramakrishnan, O. A. von Lilienfeld

**Ultrafast excited-state dynamics of the azo dye methyl orange [PC-103]**

Christoph Nançoz, University of Geneva  
B. Dereka, O. Yushchenko, J. Beckwith, R. Letrun,  
A. Rosspeintner, S. Richert, E. Vauthey

**Development of membrane mechanosensor [PC-104]**

Roberto D. Ortuso, University of Geneva  
K. Sugihara

**Rechargeable Dual Electrolytes Li-Air and Li-Water Batteries [PC-105]**

Nam Hee Kwon, University of Fribourg  
Y. Sheima, K. Fromm

**Effects of Steric Hindrance and Electron Relaxation on DNP Enhancement at High Field [PC-106]**

Dominik J. Kubicki, EPF Lausanne  
C. E. Avalos, B. Náfrádi, M. Yulikov, G. Casano, S. Abel,  
C. Sauvée, K. Ganesan, G. Jeschke, P. Tordo, A. Lesage,  
O. Ouari, L. Emsley

**Electron-Transfer Dynamics at Water-Dodecane Interface Probed by Surface Second Harmonic Generation [PC-107]**

Tatu Kumpulainen, University of Geneva  
G. Licari, A. Efimov, E. Vauthey

**Bimolecular Charge Separation and Recombination in Dipolar and Ionic Environments [PC-108]**

Arnulf Rosspeintner, University of Geneva  
G. Angulo, M. Koch, E. Vauthey

**Rydberg-Stark deceleration of metastable triplet helium atoms in a magnetic field [PC-109]**

Matija Zesko, ETH Zurich  
O. Tkáč, F. Merkt

**Orientation of a DNA probe at biological-like interfaces [PC-110]**

Giuseppe L. Licari, University of Geneva  
L. Cwiklik, P. Jungwirth, E. Vauthey

**Calorimetric and Spectroscopic Studies on the Solvation Energetics for H<sub>2</sub> Storage in the CO<sub>2</sub>/HCOOH System [PC-111]**

Cornel Fink, EPF Lausanne  
G. Laurency

**Threshold Photoelectron Spectroscopy to trace Chemistry in Combustion, Pyrolysis and Catalysis [PC-112]**

Patrick Hemberger, Paul Scherrer Institute, Villigen

**Precision Spectroscopy in Cold Molecules: The Rotational Intervals of He<sub>2</sub><sup>+</sup> by High-Resolution Spectroscopy and Rydberg-Series Extrapolation [PC-113]**

Luca Semeria, ETH Zurich  
P. Jansen, J. A. Agner, H. Schmutz, F. Merkt

**Modifying peptides and proteins for quantum interference experiments [PC-114]**

Jonas Schaetti, University of Basel  
U. Sezer, L. Mairhofer, J. Cotter, M. Arndt, V. Köhler, M. Mayor

**Gold nanowire fabrication with lipid nanotubes [PC-115]**

Kristina Jajcevic, University of Geneva  
K. Sugihara

**Determining Nano to Micro Structures from Relayed DNP NMR [PC-116]**

Arthur C. Pinon, EPF Lausanne  
J. Schlagnitweit, P. Berruyer, A. Rossini, A. Lesage, C. Copéret, L. Emsley

**Long-range molecules correlated to electronically highly excited states in Cs [PC-117]**

Heiner Sassmannshausen, ETH Zurich  
F. Merkt, J. Deiglmayr

**Cold and controlled mechanistic studies of conformer selected ionic cycloadditions [PC-118]**

Ardita Kilaj, University of Basel  
D. Rösch, H. Gao, J. Küpper, S. Willitsch

**Towards Continuous Trap Loading of Helium in Rydberg States [PC-119]**

Ondřej Tkáč, ETH Zurich  
M. Zesko, F. Merkt

**Dynamic Nuclear Polarization Method as a Probe of Lipid Nanoparticles Structure [PC-120]**

Jasmine Viger-Gravel, EPF Lausanne  
A. Schantz, A. Rossini, A. C. Pinon, S. Schantz, L. Emsley

**Collision-Induced Rotational Excitation in N<sub>2</sub><sup>+</sup>-Ar: Comparison of Computations and Experiment [PC-121]**

Oliver T. Unke, University of Basel  
J. C. Castro-Palacio, M. Meuwly

**Conformational effects in neutral and ionic Diels-Alder reactions [PC-122]**

Uxía Rivero, University of Basel  
M. Meuwly, S. Willitsch

**Unraveling the electronic states of transition metal species by optical spectroscopy [PC-123]**

Martin Beck, Paul Scherrer Institute  
B. Visser, P. Bornhauser, G. Knopp, J. A. van Bokhoven, P. P. Radi

**Two-dimensional infrared spectroscopy of a site-specifically labeled photoswitchable allosteric protein [PC-124]**

Olga Bozovic, University of Zurich  
B. Stucki-Buchli, P. J. Johnson, K. L. Koziol, P. Hamm

**Ultrafast and Nanosecond Transient Absorption and Photoluminescence Spectroscopy Enlightens the Pathway towards Perovskite Electronic and Photovoltaic Devices [PC-125]**

Nikolaos Droseros, University of Fribourg  
G. Longo, H. J. Bolink, N. Banerji

**Terahertz Emission Spectroscopy on Thin Films [PC-126]**

Philipp Krauspe, University of Fribourg  
D. Tsokkou, N. Banerji

**Photophysical study of a water-soluble cationic polythiophene derivative [PC-127]**

Lisa Peterhans, University of Fribourg  
J. C. Brauer, E. Alloa, M. Leclerc, S. C. Hayes, N. Banerji

**Possible role of triplet states in matrix-assisted laser desorption ionization investigated by time resolved decay measurements [PC-128]**

Philipp Steffen, University of Bern  
R. Knochenmuss, S. Leutwyler

**Structural studies on mixed shell thiolate-protected gold clusters [PC-129]**

Annelies Sels, University of Geneva  
N. Barrabes, T. Bürgi

**Ag doped Au<sub>38</sub>(SC<sub>2</sub>H<sub>4</sub>Ph)<sub>24</sub> nanocluster: metal migration and chiroptical properties [PC-130]**

Bei Zhang, University of Geneva  
T. Bürgi

**Wood filter technology for waste water treatment [PC-131]**

Selin Vitas, ETH Zurich  
I. Burgert, E. Cabane

**Charge Carrier Dynamics in Dye-Sensitized Solar Cells Investigated by Ultrafast Electromodulated Differential Absorption Spectroscopy [PC-132]**

Andrés Burgos, EPF Lausanne  
J.-E. Moser

**Structural models of calcium silicate hydrate nanoparticles from NMR constraints [PC-133]**

Brennan J. Walder, EPF Lausanne  
A. Kumar, A. Mohamed, B. Srinivasan, A. Hofstetter, A. Rossini, P. Bowen, K. Scrivener, L. Emsley

**Spectroscopy of H<sub>2</sub><sup>+</sup> and HD<sup>+</sup> Near the Dissociation Threshold: Shape and Feshbach Resonances [PC-134]**

Maximilian Beyer, ETH Zurich  
F. Merkt

**Encoding of chemical shifts using multiple indirect evolution in Homo- and Heteronuclear NMR experiments [PC-135]**

Eduard Sistaré, University of Geneva  
D. Jeannerat

**Evidence of spin state changes in homogeneous solar water splitting [PC-136]**

Sue Yun Oh, Empa Materials & Technology  
D. Bleiner, A. Borgschulte

**Excited state and light-induced electron injection dynamics in diketopyrrolopyrrole-based push-pull organic dye-sensitized solar cells [PC-137]**

Heewon Bahng, EPF Lausanne  
J.-E. Moser

**Ultrafast Electromodulated Absorption Spectroscopy of Perovskite Solar Cells: Investigating Charge Carrier Separation Dynamics under Externally-Applied Electric Field [PC-138]**

Arun Aby Paraecattil, EPF Lausanne  
M. Bouduban, J. De Jonghe, A. Ajdarzadeh, J. Teuscher,  
J.-E. Moser

**Electron Transfer within MAPbBr<sub>3</sub> Perovskite Colloidal Nanoparticles [PC-139]**

Marine E. F. Bouduban, EPF Lausanne  
A. Burgos, R. Ossola, J.-E. Moser

**Experimental studies of the ion-molecule reactions H<sub>2</sub><sup>+</sup> + H<sub>2</sub> and H<sub>2</sub><sup>+</sup> + D<sub>2</sub> at low collision energies with a merged beam apparatus [PC-140]**

Katharina Höveler, ETH Zurich  
P. Allmendinger, J. Deiglmayr, F. Merkt

**Computational study on the O<sub>2</sub> formation on Amorphous solid water in cold interstellar clouds [PC-141]**

Marco Pezzella, University of Basel  
O.T. Unke, M. Meuwly, M. Meuwly

**Simultaneous Optical and Electrochemical Characterization of Voltage Sensitive Dyes in Lipid Membranes [PC-142]**

Maria Tsemperouli, University of Geneva  
K. Sugihara

**Structural investigation of the HS to LS relaxation dynamics on [Fe(pz)Pt(CN)<sub>4</sub>] spin crossover nanoparticles [PC-143]**

Teresa Delgado, University of Geneva  
A. Tissot, L. Guénée, P. Pattison, A. Hauser, C. Besnard

**Solvent Suppression in DNP-Enhanced Solid State NMR [PC-144]**

Jayasubba Reddy Yarava, EPF Lausanne  
S. R. Chaudhari, A. Rossini, A. Lesage, L. Emsley

**On the formation of H<sub>2</sub><sup>+</sup> by radiative recombination [PC-145]**

Lukas Möller, ETH Zurich  
M. Beyer, F. Merkt

**NMR Studies of Hierarchical Protein Dynamics [PC-146]**

Baptiste Busi, EPF Lausanne  
J. Yarava, A. Hofstetter, M. Blackledge, L. D. Emsley

**Complex thermolysis mechanism of phosphoramidate: Formation of PN based gas phase active phosphorus species [PC-147]**

Shuyu Liang, EMPA/ETH Zurich  
P. Hemberger, J. Levalois-Grützacher, O. Korobeinichev,  
H. Grützacher, S. Gaan

**Ionic Liquids based on Crown Ethers as electrolytes for batteries [PC-148]**

Hervé Yao, University of Fribourg  
K. M. Fromm

**Time-resolved THz spectroscopy of Rhenium complex solvation in water [PC-149]**

Saima Nafees Ahmed, University of Zurich  
A. Shalit, P. Hamm

**Evaluating the magneto-crystalline anisotropy constant of (SPIONs) systems [PC-150]**

Julio Cesar Martinez Garcia, Adolphe Merkle Institute,  
Fribourg  
F. Crippa, C. A. Monier, A. M. Hirt, A. P. Fink, M. Lattuada

**Interrogating Weakly Bound Complexes by Velocity Map Imaging Photoelectron Photoion Coincidence [PC-151]**

Andras Bödi, Paul Scherrer Institut

**Halide Free M(BH<sub>4</sub>)<sub>2</sub> (M= Sr, Ba and Eu): Single Route Synthesis [PC-152]**

Manish Sharma, University of Geneva  
L. Daku, R. Černý, H. Hagemann

**Mechanism of the cooperativity in antimicrobial peptides [PC-153]**

Ewa B. Drab, University of Geneva  
K. Sugihara

**Polymers, Colloids & Interfaces [PI]  
Poster Session****Click-Thiols as an approach to implement novel functionalities within bio-derived scaffolds [PI-101]**

Sanja Kostic, ETH Zurich  
E. Cabane, I. Burgert

**LDH-polyelectrolyte nanocomposites as novel materials or enzyme carriers [PI-102]**

Marko Pavlovic, University of Geneva  
P. Rouster, I. Szilágyi

**Ag nanoencapsulation for antimicrobial implant coatings [PI-103]**

Sarah-Luise Abram, University of Fribourg  
M. Priebe, K. M. Fromm

**Development of high permittivity siloxanes for dielectric elastomer generators [PI-104]**

Philip Caspari, Empa Materials Science and Technology  
D. Opris, F. Nüesch

**Effect of aging on silica aerogel properties and study of the structure of glass wool aerogel composites by X-ray tomography [PI-105]**

Subramaniam Iswar, Empa Materials Science and  
Technology  
W. J. Malfait, M. Griffa, M. M. Koebel, M. Lattuada

**Excitation energy transfer over base pairs in DNA based light-harvesting antennae [PI-106]**

Caroline D. Bösch, University of Bern  
E. Abay, S. M. Langenegger, M. Nazari, M. Akbarimoosavi,  
M. Gazzetto, A. Rondi, A. Cannizzo, T. Feurer, R. Häner

**Surface functionalisation of titania nano-objects for biocatalytic applications [PI-107]**

Paul Rouster, University of Geneva  
M. Pavlovic, I. Szilágyi

**DNA-grafted supramolecular polymers: self-assembly, dynamics and potential applications [PI-108]**

Yuliia Vyborna, University of Bern  
R. Häner

**Effect of supramolecular interactions in dendronized polymers on their thermal- and viscoelastic properties [PI-109]**

Leon F. Scherz, ETH Zurich  
S. Costanzo, T. Schweizer, D. Vlassopoulos, A. D. Schlüter

**Layer-Controlled Colloidal Dispersions of Two-Dimensional Organometal Halide Perovskites for Efficient Blue Light-Emitting Diodes [PI-110]**

Jakub Jagielski, ETH Zurich  
S. Kumar, C. Shih

**PEGylated chelator-based calcium phosphate nanoparticles for gene delivery [PI-111]**

Xiangang Huang, ETH Zurich  
D. Andina, J.-C. Leroux, B. Castagner

**Functionalization of arrays of silica nanochannels by post-condensation [PI-112]**

Nicola Zucchetto, Zurich University of Applied Sciences, ZHAW  
D. Brühwiler

**Ferrocene derivatives: new mechanophore for stimuli-responsive materials [PI-113]**

Michela Di Giannantonio, University of Fribourg  
M. Ayer, E. Verde Sesto, C. Weder, K. Fromm

**Piezoelectric Elastomer Composites [PI-114]**

Yee Song Ko, EPF Lausanne  
F. Nüesch, D. Opris

**Solid-state NMR spectroscopy of silica and silica-biopolymer hybrid aerogel [PI-115]**

Wim J. Malfait, Empa Dübendorf  
M. M. Koebel, D. Rentsch, S. Zhao, R. Verel

**Design of poly(N-isopropylacrylamide)-silver nanocomposites for biomedical applications [PI-116]**

Milene Tan, University of Fribourg  
A. Holzheu, K. Fromm

**Ionic Conductivity and Lithium Ion Transference Number in Lithium Ion Battery Separators: Membrane Geometry versus Surface Chemistry [PI-117]**

Raphael Zahn, ETH Zurich  
M. Lagadec, M. Hess, V. Wood

**Self-Assembly of Gold Nanoparticle at Liquid-Liquid Interfaces: the Role of the Interfacial Surface Tension [PI-118]**

Evgeny Smirnov, EPF Lausanne  
P. Peljo, H. Girault

**Polar Siloxanes for Dielectric Elastomer Actuators [PI-119]**

Simon Dünki, Empa Dübendorf / EPF Lausanne  
F. Nüesch, D. Opris

**Hydrophobization of silica aerogels by mixed alkoxysilanes [PI-120]**

Ana Stojanovic, Empa Materials Science and Technology  
S. P. Comesana, W. J. Malfait, M. M. Koebel

**Water sorption behavior of physically and chemically activated monolithic nitrogen doped carbon [PI-121]**

Lukas Huber, Empa Materials Science and Technology  
P. Ruch, R. Hauert, S. Matam, G. Saucke, S. Yoon, Y. Zhang, M. M. Koebel

**Self-cleaning, reliable and accurate: new nanostructured device takes electroanalysis of neurotransmitters to the next level [PI-122]**

Guido Panzarasa, Empa Materials Science and Technology  
V. Pifferi, G. Soliveri, S. Ardizzone, L. Falciola

**Efficient Anion-Exchange in Highly Luminescent Nanocrystals of Cesium Lead Halide Perovskites (CsPbX<sub>3</sub>, X = Cl, Br, I) [PI-123]**

G. Nedelcu, ETH Zurich  
L. Protesescu, S. Yakunin, M. Bodnarchuk, M. J. Grotevent, M. V. Kovalenko

**From supramolecular to covalent Polymers *via* disulfide crosslinking [PI-124]**

Giovanni Picca, University of Bern  
R. Häner

**Study of Electrical Double Layer in Solutions of Like-Charged Polyelectrolytes Using an Atomic Force Microscopy [PI-125]**

Mohsen Moazzami Gudarzi, University of Geneva  
T. Kremer, V. Valmacco, P. Maroni, M. Borkovec, G. Trefalt

**Polystyrene sulfonate adsorption on silica induced by multivalent counterions [PI-126]**

Tomislav Kremer, University of Geneva  
A. Tiraferri, P. Maroni, M. Borkovec

**Self-Assembled Monolayer (SAM) of Cyanine Dye J-Aggregates on Surfaces for Mesoscopic Solar Cells [PI-127]**

Surendra Babu Anantharaman, EMPA, Dübendorf  
F. Nüesch, J. Heier

**Investigating partially dispersed colloidal suspensions by high-frequency rheology [PI-128]**

Bram Schroyen, ETH Zurich

**Efficient light-harvesting Antenna through the intermediate donor-acceptor pyrene derivative [PI-129]**

Mariusz Kownacki, University of Bern  
S. M. Langenegger, R. Häner

**Polymer brushes: new opportunities for their patterning and characterization [PI-130]**

Guido Panzarasa, Empa Materials Science and Technology

**Artificial lipid droplets covered by a monolayer of sphingomyelin and cholesterol [PI-131]**

Valerija Vežočanik, University of Ljubljana  
S. Sitar, K. Kogej, M. Tušek-Žnidarič, K. Sepčić, M. Šentjurs, V. Hodnik, D. Pahovnik, E. Žagar, P. Maček

**Homogeneous Synthesis of Surfactant-free Janus Nanoparticles and Its Application as Solid Amphiphilics [PI-132]**

Dalin Wu, Zurich University of Applied Sciences, ZHAW  
A. Honciuc

**Influence of particle anisotropy on cluster rigidity and rheology of colloidal gels [PI-133]**

Gabriele Colombo, ETH Zurich  
J. Vermant

**Controlled self-organisation of networks based on {M(2,2':6',2'':terpyridine)}<sup>2+</sup>-zipped co-block polymer nanocompartments [PI-134]**

Alexandra Wiesler, University of Basel  
I. A. Dinu, C. G. Palivan, E. C. Constable, C. E. Housecroft

**Wetting of rough particles at flat liquid-liquid Interfaces [PI-135]**

Michele Zanini, ETH Zurich  
C. Marschelke, A. Synytska, L. Isa

**Synthesis of amphiphilic giant hollow helices [PI-136]**

Samantha Doninelli, University of Fribourg  
M. Schulze, A. Kilbinger

**Templated polymerization using nucleobase-substituted monomers for non-covalent interactions [PI-137]**

Elodie Repond, University of Fribourg  
A. Kilbinger

**The counter-intuitive destabilizing effect of surfactant addition in a dispersion of polymer-brushed particles [PI-138]**

Tommaso Casalini, ETH Zurich  
B. Jaquet, G. Pavan, M. Morbidelli

**Enzymatic oligomerization in AOT vesicle membranes [PI-139]**

Sandra Luginbühl, ETH Zurich  
M. Willeke, L. D. Schuler, T. Ishikawa, P. Walde

**Quantification of lipid vesicle-entrapped peroxidase with *p*-phenylenediamine [PI-140]**

Ya Zhang, ETH Zurich  
S. Luginbühl, Y. R. Schmid, P. Dittrich, P. Walde

**Resonance Raman Optical Activity of Single Walled Carbon Nanotube Enantiomers [PI-141]**

Martin Magg, University of Geneva  
P. Oulevey, T. Bürgi

**Kinetic and Particle Size Considerations in Dispersion Polymerization of Methyl Methacrylate in Hexane [PI-142]**

Eric Jean Fischer, ETH Zurich  
M. Ravi, G. Storti, M. Morbidelli

**Cu-In-Te and Ag-In-Te colloidal nanocrystals with tunable composition and size [PI-143]**

Olesya Yarema, ETH Zurich  
M. Yarema, V. Wood

**Colloidal Chemistry to Advance Solar-to-Chemicals Conversion Studies [PI-144]**

Raffaella Buonsanti, EPF Lausanne

**Smart Photonic Crystals of Stimuli-responsive Microgels [PI-145]**

Golnaz Isapour, University of Fribourg  
M. Lattuada

**Ultra light nanofiber based 3D scaffolds with tunable porosity and air permeability [PI-146]**

Fabian Deuber, Zurich University of Applied Sciences, ZHAW  
S. Mousavi, C. Adlhart

**Reversible Thermoresponsive Dispersion / Aggregation of Inorganic Nanoparticles embedded in Polymer Matrix [PI-147]**

Lu Jin, ETH Zurich

**Development of functionalized hybrid hydrogels [PI-148]**

Francois Noverraz, EPF Lausanne  
S. Passemard, E. Montanari, F. Borcard, S. Gerber, C. Wandrey

**Challenges in determining the rate capability of battery materials [PI-149]**

Michael Hess, ETH Zurich  
P. Novák, V. Wood

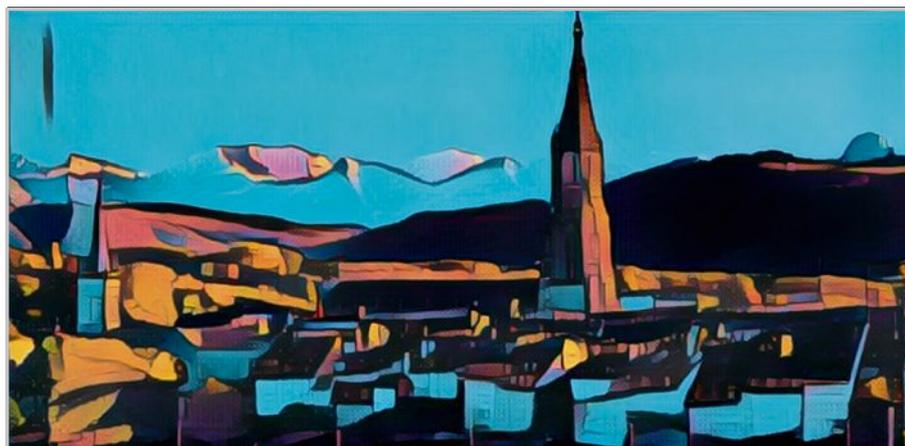
**Dendrimer decorated nylon 6 electrospun nanofibrous membranes for the efficient dye removal from waste water [PI-150]**

Sara Mousavi, Zurich University of Applied Sciences, ZHAW  
F. Deuber, F. Shahraki, C. Adlhart

**Self-organization of polymeric nano-compartments or nano-reactor-origami [PI-151]**

Samuel Lörcher, University of Basel  
J. Liu, V. Postupalenko, D. Wu, M. Chami, W. Meier, C. G. Palivan

The complete program and all abstracts are available as interactive application on <http://scg.ch/fallmeeting/2016>

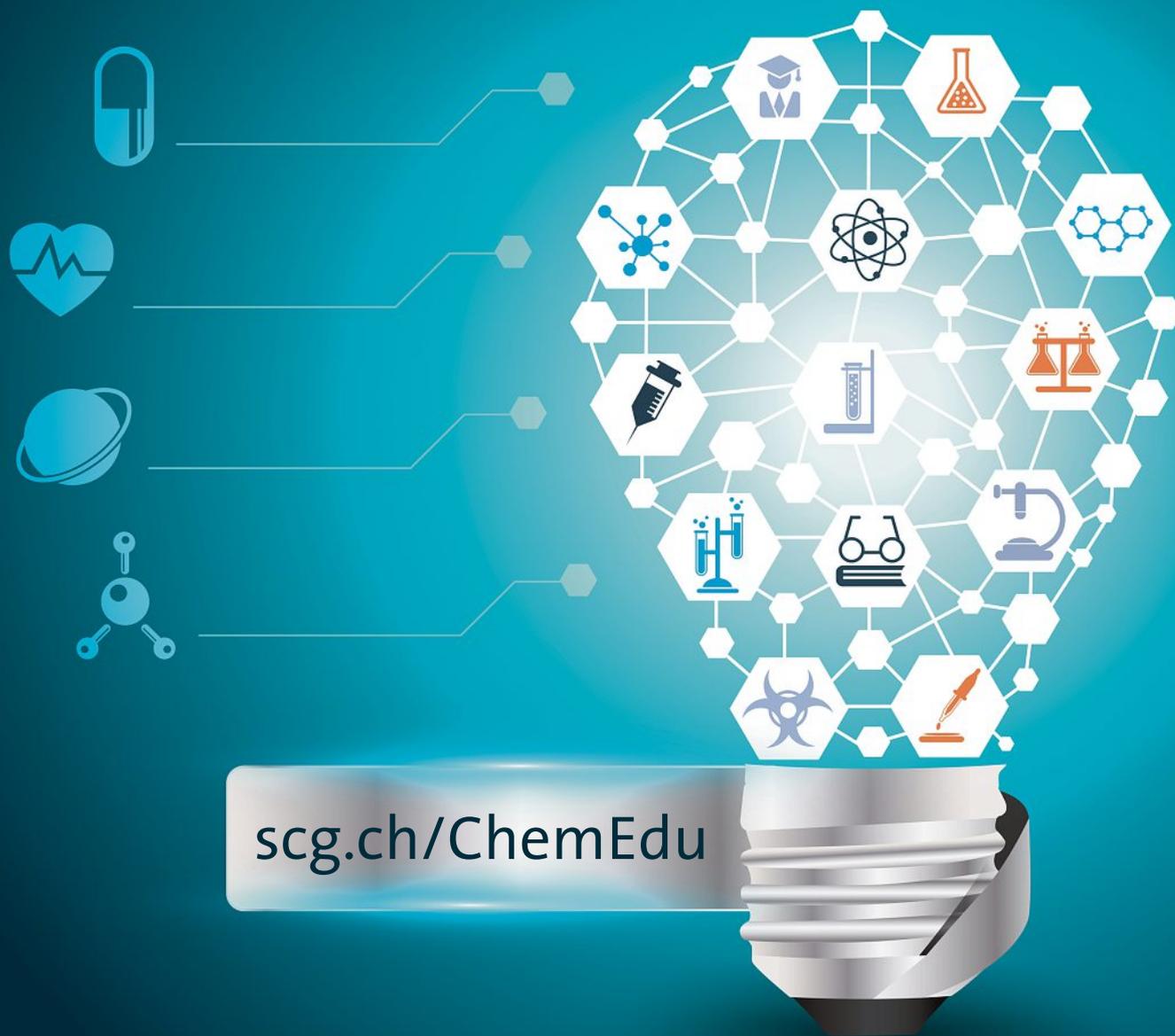


**u<sup>b</sup>**  
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**SCS**  
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**SCS Fall Meeting 2017**

University of Bern, VonRoll Areal  
21.-22. August 2017



[scg.ch/ChemEdu](http://scg.ch/ChemEdu)

# Future of Chemical Education

Symposium and Workshops

15<sup>th</sup> September 2016, 08.30–18.00  
University of Zurich, Irchel Campus



**SCS**  
Swiss Chemical  
Society

The event is part of the SCS Fall Meeting 2016 and will provide ideas and best practice in theoretical, practical and experimental chemical education and targets qualified teachers from secondary school on upwards.

## FUTURE OF CHEMICAL EDUCATION – SYMPOSIUM AND WORKSHOPS, SEP 15, 2016

Given its increasing importance, the Swiss Chemical Society (SCS) decided to extend its activities into the area of chemical education. The new Division of Chemical Education (DCE), which now is in the process of being established, shall support the interaction of educators and teachers of chemistry at all levels. The possibility to interact with scientists of the other SCS divisions will create bridges between research and education. To launch this process, the symposium 'Future of Chemical Education', which is part of the next SCS Fall Meeting, will be held at University of Zürich on September 15, 2016.

The event will provide ideas and best practice in theoretical, practical and experimental chemical education and targets qualified teachers from secondary school on upwards.

We are looking forward to an exciting event and hope to initialize a successful initiative to promote chemical education on all teaching levels.

Best regards,

Prof. Antonio Togni, ETHZ

Prof. Roger Alberto, UZH

Dr. Amadeus Bärtsch, ETHZ

Dr. Klemens Koch, VSN

Dr. Markus T. Müller, ETHZ and Kantonsschule Frauenfeld

Dr. Hans Peter Lüthi, SCS and ETHZ

### Program Overview

- 08.30 Registration, welcome coffee  
 09.00 Welcome message  
**Prof. Antonio Togni**, Laboratory of Inorganic Chemistry, ETH Zurich  
 Short welcome speech of Dr. Alain De Mesmaeker, Präsident SCS  
 09.15 **Prof. Michael Tausch**, Bergische Universität Wuppertal (GER)  
 All we need is Light – Mehr Licht im Chemieunterricht  
 10.00 **Prof. Hans Jakob Wörner**, Laboratory of Physical Chemistry, ETH Zurich  
 Attosecond Spectroscopy: Watching Electrons in Motion  
 10.45 Short break  
 11.00 **Prof. Catherine E. Housecroft**, Department of Chemistry, University of Basel  
 Development of Chemistry Textbooks – an interactive Process  
 11.45 **Prof. Wendelin Jan Stark**, Institute for Chemical and Bioengineering, ETH Zurich  
 Young Entrepreneurs in Chemistry: Getting out of the Laboratory  
 12.30 Lunch break and Poster Session of the SCS Fall Meeting  
 13.30 Workshop sessions A-D (detailed program see below)  
 17.00 Paracelsus Award Lecture (part of the SCS Fall Meeting program), **Prof. Michael Grätzel**, EPF Lausanne  
 18.30 Dinner (optional: costs CHF 50.00 for 3-course menu including beverages such as mineral water, beer, wine, coffee. To be paid at the registration desk)

### Workshop-Session A, Target level: SekI, SekII, BS

- A1 **Paolo Lubini**, Liceo Cant. Lugano 2, **Michele D'Anna**, Liceo Cant. Locarno  
 Chemisches Potential und Entropie im gymnasialen Unterricht: Warum nicht?  
 A2 **Dr. Jurai Lipscher**, Ruppertswil  
 Der Klimawandel – Was wissen wir wirklich?  
 A3 **Prof. Roger Alberto**, University of Zurich, Dr. Urs Leutenegger, KS Zug  
 Artificial Photosynthesis\*

- A4 **Giorgio Zambrino**, KS Enge, **Lukas Sigrist**, ETH Zürich  
 Chemische Reaktionen in Super-Slow-Motion

### Workshop-Session B, Target level: FH, PH, HS

- B1 **Prof. Carlo Thilgen**, ETH Zürich, **Prof. Bernhard Jaun**, ETH Zürich  
 Der Einsatz von Moodle in den Vorlesungen OC1 & OC2 (Übungen, Training, Prüfungen?)\*  
 B2 **Niels Sievertsen**, ETH Zürich  
 Die ganze Organische Chemie in der Hosentasche – Advanced Problems in Organic Chemistry (apoc) at Students' Fingertips  
 B3 **Dr. Markus T. Müller**, KS Frauenfeld, **Prof. Antonio Togni**, ETH Zürich, **Prof. Carlo Thilgen**, ETH Zürich  
 Schnittstelle Mittelschule–Hochschule am Beispiel AC1 und OC1 – Standortbestimmung AC1/OC1 HS 2015 & 2016

### Workshop-Session C, Chemielabor und Praktikum

- C1 **Prof. Michael W. Tausch**, Bergische Universität Wuppertal  
 Photo-Blue-Bottle – Modellexperimente zum Kreislauf Photosynthese–Atmung  
 C2 **Dr. Robert Grass**, ETH Zürich  
 Nanotechnologie und funktionelle Polymere im Unterricht  
 C3 **Franziska Krieg** et. al, ETH Zürich, **Prof. Maksym V. Kovalenko**, ETH Zürich  
 Einfache Synthese von stark fluoreszierenden Caesium-Blei-Halogenid-Perovskit-Nanokristallen – Ein farbenfrohes Chemiepraktikum für die Mittelschule  
 C4 **Dr. Hansrudolf Dütsch**, Zürich  
 Leuchtstab (Knicklicht) und Synthese eines chemilumineszierenden Oxalsäureesters TCPO  
 C5 **Pitt Hild**, PH Zürich  
 Tagescreme oder Nachtcreme? Emulsionen im Unterricht

### Workshop-Session D, Computerraum (Visualisierung, Animation, Simulation)

- D1 **Dr. Moritz Haag**, ETH Zürich, **Alain Vaucher**, ETH Zürich, **Prof. Markus Reiher**, ETH Zürich  
 Interactive Exploration of Chemical Reactivity in Education (3D-Modellierung chemischer Reaktionen)  
 D2 **Dr. Marie-Claude Blatter**, **Dr. Antoine Daina**, **Dr. Vincent Zoete**, Swiss Inst. of Bioinformatics, Geneva  
 Computer-Aided Drug Design explained in a few simple steps (Drug Design Workshop)  
 D3 **Dr. Hans Ueli Ehrensperger**, Frauenfeld  
 Visualisierung im Chemieunterricht – das Atomarium und andere Leckerbissen  
 D4 **Dr. Urs Leisinger**, KS Zug  
 Visualisierung von Molekülen im Chemieunterricht mit JSmol – www.molek.ch  
 D5 **Marcel Ottiger**, Hedingen  
 Neuauflage der „Kurt Pfefferkorn“-Animationen für den Chemieunterricht  
 \* working titles, to be confirmed

The full program incl. abstracts are available on the website.  
<http://scg.ch/chemedu/2016>

Registration deadline is August 31, 2016. The event is free for SCS members and costs CHF 50.00 for non-SCS members.

### Contact

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ab Mitte August 2016:

Kantonsschule

Speicherstrasse 10

8500 Frauenfeld