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, EPFL Lausanne,
18.00 Best Presentation Award Ceremonies
18.30 End of the conference

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

Electronic structure and reactivity of hypervalent iodine reagents. Credit: H.Pinto de Magalhães, A. Togni Group, ETH Zürich.
**Welcome to the 2016 Fall Meeting of the Swiss Chemical Society (SCS)**

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!

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**

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
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 19th 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.[1]

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.

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!

**Program Overview**

Interactive program incl. all abstracts of the lectures, talks and posters on [http://scg.ch/fallmeeting](http://scg.ch/fallmeeting)

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<td>Dr. Martin Weibel, Dr. Robert Flatt, Dr. Hendrik Heinz, Sika Technology AG</td>
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<td>«Development of commercial organic additives for the grinding of inorganic solids» [PS-002]</td>
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<td>Prof. Michael Graetzel, École Polytechnique Fédérale de Lausanne, EPFL,</td>
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<td>«Invention and development of the dye-sensitized solar cells» [PS-003]</td>
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<td>18.00</td>
<td>Best Oral Presentation Awards (sponsored by Metrohm)</td>
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<td>Presented by Dr. Volker Frost, Metrohm AG</td>
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<td>18.15</td>
<td>Best Poster Presentation Awards (sponsored by DSM)</td>
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<td>Presented by Dr. Roman Imhof, DSM Nutritional Products Ltd.</td>
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<td>End of the conference</td>
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**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](http://scg.ch/fallmeeting)

**Chairman**  
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**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](http://scg.ch/membership).

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

**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.

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**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)
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.

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

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. Koptyug (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)
– 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

Ceremony of the Best Poster Presentation Award at EPFL 2015
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

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

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

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.com

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

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

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

Contact Group for Research Matters (KGF)
General Sponsor 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

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

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

Swiss Academy of Science, Platform Chemistry
General Meeting Sponsor
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

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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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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 Chemical 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 additives 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 University 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 optically 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 racemic compounds on optically active polymers as chiral stationary phases and his pioneering work in implementing 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 Industrial Polymer».  
Session of Polymers, Colloids & Interfaces, [PI-011], lecture hall G55.  
The award is given for Prof. Nesvadba’s groundbreaking 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 Chemistry Approach?»  
Session of Medicinal Chemistry & Chemical Biology [MC-012], lecture hall G60.  
The award is given for Dr. Bolli’s excellent contributions in medicinal chemistry culminating in the discovery 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 contributions to make profragrance chemistry an interdisciplinary 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.

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  

### Analytical Sciences [AS]

**Morning Session – G95**  
Chair: Dr. Hanspeter Andres

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<tr>
<td>11.15</td>
<td>Chromatographic resolution of racemic compounds on optically active polymers as chiral stationary phases [AS-011]</td>
<td>Eric Francotte, Novartis Institutes for Biomedical Research</td>
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<td>11.45</td>
<td>Towards a better understanding of spectral similarity between structurally related compounds [AS-013]</td>
<td>Jennifer E. Schollée, Eawag, Dübendorf (J. Hollender)</td>
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<td>12.00</td>
<td>Understanding the cellular distribution and protein targets of a ruthenium (II) anti-cancer compound, RAPTA-T via mass spectrometry [AS-014]</td>
<td>Ronald F. S. Lee, EPF Lausanne (P. J. Dyson)</td>
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<td>12.15</td>
<td>Combined GC- and UHPLC-HR-MS based metabolomics to analyze durable anti-fungal resistance processes in cereals [AS-015]</td>
<td>Rahel Bucher, University of Zurich (B. Keller)</td>
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**Afternoon Session – G95**  
Chair: Dr. Stefan Schürch

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<td>15.15</td>
<td>Electrochemical Proton Transfer Based Polyani-line Films for Thin Layer Titrations [AS-022]</td>
<td>Majid Ghahraman Afshar, University of Geneva (E. Bakker)</td>
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<td>15.30</td>
<td>Persistent organic pollutants in white-blooded Antarctic fish <em>Champsocephalus gunnari</em> and <em>Chaenocephalus aceratus</em> [AS-023]</td>
<td>Markus Zennegg, Empa</td>
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<td>15.45</td>
<td>Field-scale <em>in situ</em> analysis of ambient N2O isotopic composition to trace source processes in an intensively managed grassland [AS-024]</td>
<td>Erkan Ibraim, Empa (J. Mohn)</td>
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<td>16.00</td>
<td>At the interface between climate research and metrology: Gas adsorption and desorption on high pressure standard cylinders [AS-025]</td>
<td>Ece Satar, University of Bern Physics Institute (H. Andres)</td>
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<td>16.30</td>
<td>Studies on discrete samples using a microdroplet generator combined with ICP-Time-of-Flight Mass Spectrometry [AS-027]</td>
<td>Lyndsey Hendriks, ETH Zurich (D. Günther)</td>
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### Computational Chemistry [CC]

**Morning Session – G91**  
Chair: Dr. Ivano Tavernelli

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<td>Industrial Impact of Computational Chemistry and Materials Science [CC-011]</td>
<td>Erich Wimmer, Materials Design s.a.r.l.</td>
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<td>12.00</td>
<td>A fast scheme for approximated Fock exchange potentials in plane wave implementations of Kohn-Sham Density Functional Theory [CC-014]</td>
<td>Martin Bircher, EPF Lausanne (U. Röthlisberger)</td>
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<td>12.15</td>
<td>Quantitative Reaction Energies from an Automated Multi-Configurational Approach [CC-015]</td>
<td>Christopher Stein, ETH Zurich (M. Reiher)</td>
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**Afternoon Session – G91**  
Chair: Dr. Marcella Iannuzzi

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<td>Industrial modeling aspects of 1,3-dicarbonyl compounds [CC-021]</td>
<td>Christoph Taeschler, Lonza AG</td>
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<td>15.30</td>
<td>Is oxide hydrogenation equivalent to reduction? Fundamental differences between TiO$_2$ and Al$_2$O$_3$ from DFT [CC-023]</td>
<td>Clelia Spreafico, ETH Zurich (J. VandeVondele)</td>
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<td>15.45</td>
<td>Interatomic many-body representation improves molecular machine learning models [CC-024]</td>
<td>Bing Huang, University of Basel (O. Lilienfeld)</td>
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<td>16.00</td>
<td>Reactive Molecular Dynamics and Infrared Spectra of Double Proton Transfers with Coupling Effects [CC-025]</td>
<td>Zhen-Hao Xu, University of Basel (M. Metzly)</td>
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<td>16.30</td>
<td>Dry Reforming and Competitive Reactions on Ni, Pd and Pt metal Surfaces from DFT Calculations and Microkinetic Modeling Simulations [CC-027]</td>
<td>Aleix Comas-Vives, ETH Zurich</td>
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<td>11.15</td>
<td>In situ Studies on the Behavior of Metal/Oxide Catalysts during the Water-gas Shift Reaction [CE-011]</td>
<td>José A. Rodriguez, Brookhaven National Laboratory, USA</td>
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<td>11.45</td>
<td>Parahydrogen-based hypersensitive NMR/MRI toolkit for catalysis [CE-013]</td>
<td>Igor V. Koptyug, International Tomography Center, Novosibirsk, Russia</td>
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<td>A closure to the controversy around hydrogen spillover: a nanolithography and single nanoparticle spectro-microscopy approach [CE-015]</td>
<td>Waiz Karim, ETH Zurich/PSI Villigen (J. A. van Bokhoven)</td>
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<td>12.45</td>
<td>Why Size Matters and Favors CO Activation on Larger Ru Nanoparticles: A Molecular Understanding from First Principles [CE-017]</td>
<td>Lucas Foppa, ETH Zurich (C. Copéret)</td>
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<td>Modelling the Phosphorous Dynamics of Vanadyl Pyrophosphate Catalysts [CE-021]</td>
<td>Gerhard Mestl, Clariant Produkte (Deutschland) GmbH</td>
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<td>15.30</td>
<td>On purpose CO production via methane oxychlorination over heterogeneous catalysts [CE-023]</td>
<td>Vladimir Paunovic, ETH Zurich (J. Pérez-Ramírez)</td>
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<td>15.45</td>
<td>Rational design of ceria-based supported noble metal catalysts for low temperature CO oxidation using transient X-ray absorption spectroscopy [CE-024]</td>
<td>René Kopelent, Paul Scherrer Institute, Villigen (O. V. Safonova)</td>
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<td>16.00</td>
<td>Titania nanocontainers and nanospheres as photocatalysts for CO2 reduction and photoelectrochemical water splitting: Structural modification [CE-025]</td>
<td>Nelly Héroult, University of Fribourg (K. M. Fromm)</td>
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<td>16.15</td>
<td>Understanding of the role of Fe in highly active and stable Ni-Fe dry reforming catalysts [CE-026]</td>
<td>Sung Min Kim, ETH Zurich (C. Müller)</td>
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<td>16.30</td>
<td>Chemical layer deposition of porous alumina overcoats increases activity and stability in liquid phase catalytic conversion of biomass-derived chemicals [CE-027]</td>
<td>Florent Héroguel, EPF Lausanne (J. Luterbacher)</td>
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<td>11.15</td>
<td>Natural Born Catalysts: Photocatalytic Water Oxidation by Molecular Metal Oxides [IC-011]</td>
<td>Marcella Bonchio, University of Padova, Italy</td>
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<td>Silver(t) N-heterocyclic complexes for C–C bond activation of alkylnitriles and catalytic application in oxazoline synthesis [IC-014]</td>
<td>Rachael Heath, University of Bern (M. Albrecht)</td>
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<td>12.15</td>
<td>C–H Activations Catalyzed by Transition-Metal Ions Isolated on Metal Oxide Surfaces [IC-015]</td>
<td>Deven Paul Estes, ETH Zurich</td>
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<td>12.30</td>
<td>Exploring Trifluoromethylthioethers as ligands – Platinum(II) complexes of 8-(trifluoromethylthio) quinoline [IC-016]</td>
<td>Carl Philipp Rosenau, ETH Zurich (A. Togni)</td>
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<td>d-Glucose-Platinum(II) Conjugates for Targeted Delivery of Platinum to Cancer Cells [IC-021]</td>
<td>Malay Patra, Massachusetts Institute of Technology / University of Zurich (S. J. Lippard)</td>
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<td>15.15</td>
<td>Red-light activated photoCORMs of Mn(II) species bearing symmetric substituted 2,2’-azopyridines [IC-022]</td>
<td>Emmanuel Kottelat, University of Fribourg (F. Zobi)</td>
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<td>15.30</td>
<td>Not so similar after all. Fundamental differences in reactivity of fac-[M(solvent)(CO)₃]+ (M = Re, ⁹⁹Tc) with CO [IC-023]</td>
<td>Angelo Frei, University of Zurich (R. Alberto)</td>
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<td>15.45</td>
<td>Controlling architecture of coordination cages via the aspect ratio of the ligands [IC-024]</td>
<td>Suzanne Maria Jansze, EPF Lausanne (K. Severin)</td>
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<td>16.00</td>
<td>Design Approaches to Blue and White Light Emitting Gold(III) Complexes [IC-025]</td>
<td>Michael Bachmann, University of Zurich (K. Venkatesan)</td>
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<td>16.15</td>
<td>Anthracene-based ligands for new luminescent coordination polymers [IC-026]</td>
<td>Serhii Vasylyevskiy, University of Fribourg (K. Fromm)</td>
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<td>16.30</td>
<td>Beyond size effects: composition-tunable properties for quaternary Cu-Zn-In-Se quantum dots [IC-027]</td>
<td>Maksym Yarema, ETH Zurich (V. Wood)</td>
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### Medicinal Chemistry & Chemical Biology [MC]
**Morning Session – G60**
Chair: Dr. Yves Auberson

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<td>Business Update SCS Division of Medicinal Chemistry and Chemical Biology [MC-011]</td>
<td>Yves Auberson, Novartis Pharma AG</td>
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<td>11.45</td>
<td>Deciphering the catalytic mechanism of the sulfoxide synthase EgtB [MC-013]</td>
<td>Kristina Goncharenko, University of Basel (F. P. Seebeck)</td>
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<td>12.00</td>
<td>Discovery and Development of the Highly Potent, Highly Selective Cathepsin S Inhibitor RG7625 for the Treatment of Autoimmune Diseases [MC-014]</td>
<td>Wolfgang Haap, F. Hoffmann-La Roche AG</td>
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<td>12.15</td>
<td>A sticky interaction: Optimizing the hydrophobic stacking between the tyrosine gate of the bacterial lectin FinH with antagonists [MC-015]</td>
<td>Brigitte Fiege, University of Basel (T. Maier)</td>
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<td>12.30</td>
<td>The discovery of a potent and orally available DotIL inhibitor [MC-016]</td>
<td>Frédéric Stauffer, Novartis Pharma AG</td>
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### Afternoon Session – G60
Chair: Prof. Jean-Louis Reymond

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<td>15.00</td>
<td>Optimization of 1,4-Disubstituted Benzodiazepines as Selective and Brain Penetrant Triple Calcium T-Channel Blockers [MC-021]</td>
<td>Romain Siegrist, Actelion Pharmaceuticals Ltd.</td>
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<td>15.15</td>
<td>A FUC/LecB system to crystallize versatile nucleic acid structures [MC-022]</td>
<td>Pascal Röthlisberger, Institut Pasteur (M. Hollenstein)</td>
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<td>15.30</td>
<td>Synthesis and oomycete fungicidal activity of a new family of inhibitors targeting an oxysterol binding protein [MC-023]</td>
<td>Martin Pouliot, Syngenta Crop Protection</td>
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<td>16.00</td>
<td>High Kinetic Stability of T-Hg(^{19})-T and DNA Polymerase Inhibition [MC-025]</td>
<td>Olivia Paula Schmidt, University of Zurich (N. W. Luedtke)</td>
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<td>16.15</td>
<td>Discovery of a Potent and Selective Reversible BTK Inhibitor for the Treatment of Autoimmune Diseases [MC-026]</td>
<td>Robert Pulz, Novartis Institutes for Biomedical Research</td>
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### Organic Chemistry [OC]
**Morning Session – G45**
Chair: Prof. Cristina Nevado

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<td>11.15</td>
<td>Profragrance chemistry as interdisciplinary research area and key technology for fragrance delivery [OC-011]</td>
<td>Andreas Herrmann, Firmenich SA</td>
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<td>11.45</td>
<td>Helically Chiral Open-Shell Polycyclic Aromatic Hydrocarbons [OC-013]</td>
<td>Prince Ravatar, University of Basel</td>
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<td>12.00</td>
<td>Chiral Ruthenium-cyclopentadienyl Complexes as Versatile Catalysts for Enantioselective Transformations [OC-014]</td>
<td>David Kossler, EPF Lausanne</td>
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### Afternoon Session – G45
Chair: Prof. Olivier Baudoin

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<td>15.00</td>
<td>Optimization of Manganese Coupling Reaction for Kilogram-scale Preparation of two Aryl-1,3-dione Building Blocks [OC-021]</td>
<td>Tomas Smejkal, Syngenta Crop Protection AG</td>
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<td>15.30</td>
<td>Mechanosensitive Fluorescent Membrane Probes [OC-023]</td>
<td>Quentin Verolet, University of Geneva (S. Matile)</td>
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<td>15.45</td>
<td>Metal-Catalyzed Stereoselective Dicarbofunctionalization of Alkynes [OC-024]</td>
<td>Andrés García-Domínguez, University of Zurich</td>
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<td>16.00</td>
<td>Development and applications of C(sp(^3))–H Alkenylation [OC-025]</td>
<td>David Dailler, University of Basel (O. Baudoin)</td>
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<td>16.30</td>
<td>Size-controlled nanoparticle formation in aqueous media with a thiol-free tripeptide [OC-027]</td>
<td>Stefano Corrà, ETH Zurich</td>
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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 CBr4 [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 13C 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, ETH Zurich (C. Copéret)

16.00  Direct visualization of excited-state symmetry breaking by ultrafast time-resolved infrared spectroscopy [PC-025]
Bogdan Derea, 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-stimuil responsive films designed through layer-by-layer assembly of PAA-b-PNIPAM block copolymers for biomedical applications [PI-014]
Alina Ospyova, 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 polyphenylene sulfide 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. Morbidelli)

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)
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. Hibiti, J. Schaefer, C. Frydmann, D. Suckau, A. Plückthun, 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]
Lorenzo Querci, ETH Zurich
B. Hattendorf, D. Günther

Investigation of the 85Rb+-88Sr+ Signal Separation by Online Electrothermal Vaporization in a fs-LA-ETV-SCICPMS Set-Up [AS-107]
Hale Ceren Yilmaz, ETH Zurich
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Manuel R. Mazenauer, Zurich University of Applied Sciences, ZHAW
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M. Ruiz, C. Cirelli, D. Bleiner

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Simone Schalles, Empa Materials Science and Technology

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Marie Humbert-Droz, University of Geneva
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Jian-Hao Li, EPF Lausanne
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Benzonitrile as a Potent and Sensitive Spectroscopic Probe for Protein Interiors [CC-116]
Padmabati Mondal, University of Basel
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Improving the exploration of free energy landscapes at the electronic structure levels [CC-117]
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Marta Da Silva Perez, EPF Lausanne

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Konstantin Karandashev, EPF Lausanne
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Michael A. Stravs, Eawag, Dübendorf
F. Pomati, J. Hollender

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Krystel El Hage, University of Basel
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Renato Figi, Empa Materials Science and Technology
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Thibaud von Erlach, EPFL Lausanne
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Esra Bozkurt, EPFL Lausanne
R. Hovius, T. A. Soares, U. Röthlisberger

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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

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Dorothea Golze, University of Geneva
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Marcella Iannuzzi-Mauri, University of Zurich
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Csaba Fábri, ETH Zurich
L. Horný, M. Quack

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Halua Pinto de Magalhães, ETH Zurich
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Lukas Reith, University of Zurich
K. Lienau, R. Moré, D. Cook, R. Walton, Y. Wu, G. R. Patzke

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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]
Ilia Moroz, ETH Zurich
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Microbial fuel cell triple stack characteristics [CE-105]
Marc Sgounx, HES-SO Valais
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Maxime Blatter, HES-SO Valais
M. Sgounx, C. Comninellis, K. Nealson, F. Fischer

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

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

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. Koptyug, C. Copéret

Dry-reforming of methane over bimetallic Ni-M/La2O3 (M = Co, Fe): The effect of the rate of La2O3 formation and phase stability on the catalytic activity and stability [CE-114]
Athenasia Tsoukalou, ETH Zurich
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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
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Kim Larmier, ETH Zurich
S. Tada, A. Comas-Vives, W.-C. Liao, C. Copéret

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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
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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
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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 CO2 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

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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

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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 CO2 [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
Q. Imtiaz, C. R. Müller, 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]
Zhiquiang 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

Monitoring pore evolution during the detemplation of zeolite catalysts by positron annihilation spectroscopy [CE-140]
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CO activation on supported Pt single-atom catalysts: a density functional theory study [CE-141]
Xing Wang, ETH Zurich/PSI Villigen
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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 Spinelld and Doped Manganese Oxides as Water Oxidation Catalysts [CE-143]
Michael Olah, University of Zurich
G. R. Patzke

Catalyst design for methane oxhalogenation – 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

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

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

Synthesis and Photocatalytic Water Oxidation Study of New Co O4 Cubane Complexes [CE-152]
Fangyuan Song, University of Zurich
G. R. Patzke

Circularly permutated and chimeric streptavidins as scaffolds for artificial metalloenzymes [CE-153]
Michela M. Pellizzoni, University of Basel

Activity Improvement by Immobilization and Protection of Artificial Imine Reductase on Silica Nanoparticles [CE-154]
Martina Ribar Hesterovicá, 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 Bártsc, ETH Zurich
R. Solarska, M. Sarnowska, O. Krysiak, J. Augustynski, M. Niederberger

Upregulation of an Artificial Zymogen by Proteolysis [CE-156]
Vincent Lebrun, University of Basel

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

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 CO2 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. Nachttegaal, T. Schildhauer, C. Copéret

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

Pressure induced chemisorption in isoreticular Metal Organic Frameworks [IC-102]
Piero Macchi, University of Bern
A. Lanza, N. Casali, 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)]^2+ 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. Guéhéne, H. Nozary, A. Hauser, C. Pighuet

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 CO₂-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 Bi₃O₅CO₃ [IC-113]
René Moré, University of Zurich
M. Olah, Y. Zhou, G. R. Patzke

New Light Emitting Electrochemical Cells with halogen containing [Cu(N^N)(P^P)][PF₆] complexes [IC-114]
Fabian Brunner, University of Basel
S. Keller, A. Pertegáš, 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. Reiker,
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. Guéhéne, H. Nozary, S. V. Eliseeva, S. Petoud,
A. Hauser, C. Pighuet

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. Precimone, 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. Laurenczy

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

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Annika Büttner, University of Basel
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Fabian Brockmeyer, Northeastern University Boston
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V. Pifferi, G. Soliveri, S. Ardizzone, L. Falcìola

Efficient Anion-Exchange in Highly Luminescent Nanocrystals of Cesium Lead Halide Perovskites (CsPbX₃, X = Cl, Br, I) [PI-123]
G. Nedelcu, ETH Zurich
L. Proteescu, S. Yakunin, M. Bodnarchuk, M. J. Groeente, M. V. Kovalenko

From supramolecular to covalent Polymers via disulfide crosslinking [PI-124]
Giovanni Picca, University of Bern
R. Hämmer

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. Valnacco, 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. Hämmer

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 Vezočnik, University of Ljubljana

Homogeneous Synthesis of Surfactant-free Janus Nanoparticles and Its Application as Solid Amphiphiles [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 $(M(2,2’;6’,2’’;terpyridine))₃$–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. Killbinger

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. Lugimbühl, 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-compartment 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
Future of Chemical Education
Symposium and Workshops

15th September 2016, 08.30–18.00
University of Zurich, Irchel Campus

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,
Dr. Hans Peter Lüthi, SCS and ETHZ
Dr. Markus T. Müller, ETHZ and Kantonsschule Frauenfeld
Dr. Hans Rudolf Dütsch, Canton of Zug

**Program Overview**

08.30 Registration, welcome coffee
09.00 Welcome message
  Prof. Antonio Togni, Laboratory of Inorganic Chemistry, ETH Zürich
  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. Jurali Lipscher, Rupperswil
  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
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-Peroxid-Nanokristallen – Ein farbenfrohes Chemiepraktikum für die Mittelschule
C4 Dr. Hansruddolf Dütsch, Zürich
  Leuchtstab (Knicklicht) und Synthese eines chemilumineszierenden Oxalsäureesters TCPO
C5 Pitt Hilt, 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 Reih, 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
  Neuausgabe 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](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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