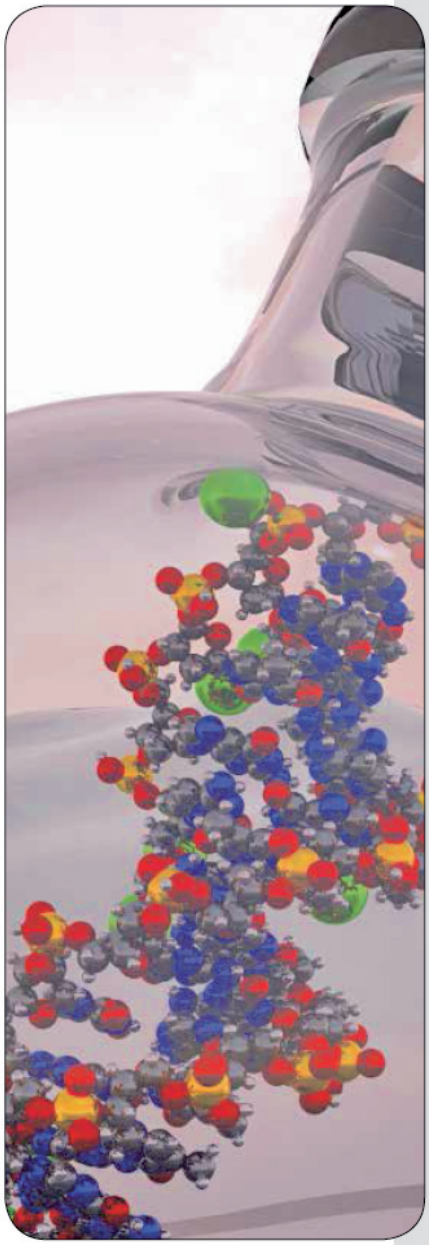

Picture by Anne-Clémence Corminboeuf, Riccardo Petraglia and Laurent Vannay, Institute of Chemical Sciences and Engineering, EPFL.

Ecole Polytechnique Fédérale
de Lausanne, EPFL
CH-1015 Lausanne

SCS
Swiss Chemical
Society

Fri, 4 September 2015, 09.00 – 18.30

SCS Fall Meeting 2015

09.45	Welcome and conference opening
09.55	Sandmeyer Award Lecture 2015 *Dr. Stefan Abele*, Actelion Pharmaceuticals Ltd «Daring the Challenge and Thinking Big: the Value of Early Process Research»
10.25	KGF-SCS Senior Industrial Science Award Lecture 2015 *Dr. Michelangelo Scalone*, F. Hoffmann La Roche «The Importance of Catalysis in the Synthesis of Active Pharmaceutical Intermediates»
11.15	Morning Parallel Session (6 slots in 8 sessions)
12.45	Lunch and Poster Session, Commercial Exhibition
15.00	Afternoon Parallel Session (8 slots in 8 sessions)
17.15	KGF-SCS Distinguished Industrial Science Award Lecture 2015 *Dr. Jürg Zimmermann*, Novartis Pharma AG «Evolution in Medicinal Chemistry»
18.00	Best Oral Presentation Awards (sponsored by Metrohm)
18.15	Best Poster Presentation Awards (sponsored by DSM)

http://scg.ch/fallmeeting/2015/

Hosted by EPFL
Institute of Chemical Sciences
and Engineering

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

doi:10.2533/chimia.2015.448 Chimia 69 (2015) 448–473

Welcome to the SCS Fall Meeting 2015

Sandrine Gerber

Christian Bochet

On behalf of the Division of Chemical Research of the Swiss Chemical Society, we warmly welcome you to the SCS Fall Meeting 2015 which will be hosted by the EPFL on its Lausanne Campus. With more than 520 scientific contributions (posters, contributed lectures, invited lectures), it is a major event for chemical researchers in Switzerland and brings together all the actors of the chemistry scene, from the starting graduate student to the seasoned senior scientist, from both academia and industry. As in the past meetings, there will be a jury to select the best oral and poster presentations for which prizes, sponsored by Metrohm and DSM, will be awarded.

Following our longtime tradition, we will have a series of invited lectures presented by distinguished scientists. This year's Sandmeyer Award Lecture will be given by Dr. Stefan Abele (Actelion Pharmaceuticals Ltd). The KGF-SCS Distinguished Industrial Investigator and Senior Industrial Investigator award lectures will be delivered by Drs. Jürg Zimmermann (Novartis Pharma AG) and Michelangelo Scalone (F. Hoffmann La Roche). Other invited and award lectures, including the Grammaticakis-Neumann Award Lecture, will be delivered in the Parallel Sessions.

The Poster Session is planned in the early afternoon, but you are welcome to visit the area at any time, in particular during the lunch and coffee breaks. Do not forget to visit the Commercial Exhibition where more than fifteen companies will be presenting their products and services.

We are very grateful to the companies and institutions who support this meeting. This support is also an expression of the interest of industry in our research activities, many of which are carried out by young scientists. The organization of such a large meeting would not be possible without the help from many people and the logistic support provided by the EPFL; we would like to thank them for their contribution to the success of this event.

We invite you to browse through the program and hope that the 2015 Fall Meeting will capture your interest. The conference tool will allow you to access the titles and abstracts through the Web. The tool also allows you to search the entries by author name and topic.

We look forward to seeing you at EPFL on September 4! Your contribution and your presence are what make this event a continuously growing success!

Prof. Christian Bochet
Chairman of the Division of Chemical Research

Prof. Sandrine Gerber
Chair of the Organizing Committee

To the Participants of the Fall Meeting of the Swiss Chemical Society

Paul J. Dyson

As you are aware, chemistry and chemical engineering are of immense value to the Swiss economy, as well as to human wellbeing. Some of the world's top chemical and pharmaceutical companies and university chemistry departments are based in Switzerland. The Swiss Chemical Society is the organ that helps to connect and inform chemists and chemical engineers working across Switzerland and its annual Fall Meeting remains the major networking event of the year. Students, postdocs and researchers from all over Switzerland and beyond meet to present and discuss their latest research. As you would expect, this meeting is only made possible thanks to the hard work of many people, who take on the various tasks in addition to their regular duties and obligations. In particular, I would like to express my thanks to the Institute of Chemical Sciences and Engineering (ISIC) administration and all the ISIC staff in our various platforms and research groups who have done so much to make the event a success. This includes personnel based at the new ISIC Valais campus in Sion.

I hope you enjoy the Fall Meeting hosted at the EPFL. Despite the frenetic pace of the day, if you get a chance take a look at the SwissTech Congress Center on the EPFL campus, which displays a 300 m^2 dye-sensitized solar cell façade. Although this technology was inspired by biology, it was invented by a physical chemist at EPFL, Prof. Michael Grätzel, and the technology now goes beyond chemistry to the realms of architecture and art. It is a wonderful demonstration of how chemists can change the world! I hope you will be inspired by the solar façade and, of course, by the seminars, posters, discussions, new ideas and contacts discovered at the Fall Meeting.

Prof. Paul J. Dyson
Director of the Institute of Chemical Sciences and Engineering (ISIC) at the EPFL

Program Overview

Interactive program incl. all abstracts on *http://chemistrycongresses.ch*

Time	Program		Lecture hall
09.00	Welcome Coffee Registration and poster installation		CE
09.45	Welcome and conference opening Prof. ***Sandrine Gerber,*** Chair SCS Fall Meeting Prof. ***Paul Dyson,*** EPFL Lausanne Prof. ***E. Peter Kündig,*** SCS President		CE 6
09.55	Sandmeyer Award Lecture 2015 [PS-001] Dr. ***Stefan Abele,*** Actelion Pharmaceuticals Ltd «Daring the Challenge and Thinking Big: the Value of Early Process Research»		CE 6
10.25	KGF-SCS Senior Industrial Science Award Lecture 2015 [PS-002] Dr. ***Michelangelo Scalone,*** F. Hoffmann La Roche «The Importance of Catalysis in the Synthesis of Active Pharmaceutical Intermediates»		CE 6
11.15	***Morning Parallel Session***		
	Analytical Sciences	[AS-011], [AS-014] … [AS-016]	CE 5
	Catalysis Science & Engineering	[CE-011], [CE-013] … [CE-016]	CE 2
	Computational Chemistry	[CC-011], [CC-013] … [CC-016]	CE 105
	Inorganic & Coordination Chemistry	[IC-011], [IC-014] … [IC-016]	CE 3
	Medicinal Chemistry & Chemical Biology	[MC-011] ... [MC-016]	CE 6
	Organic Chemistry	[OC-011] … [OC-016]	CE 1
	Physical Chemistry	[PC-011], [PC-013] … [PC-016]	CE 4
	Polymers, Colloids & Interfaces	[PCI-010], [PCI-012], [PCI-014] … [PCI-017]	BS 160
12.45	Lunch and Commercial Exhibition		CE/BS
	Poster Session		
	Analytical Sciences	[AS-101] … [AS-136]	CE 100
	Catalysis Science & Engineering	[CE-101] … [CE-160]	CE 106
	Computational Chemistry	[CC-101] … [CC-130]	CE 102
	Inorganic & Coordination Chemistry	[IC-101] … [IC-163]	CE 103
	Medicinal Chemistry & Chemical Biology	[MC-101] … [MC-160]	SPO
	Organic Chemistry	[OC-101] … [OC-164]	SPO
	Physical Chemistry	[PC-101] … [PC-154]	CE 101
	Polymers, Colloids & Interfaces	[PCI-101] … [PCI-148]	BS 170
15.00	***Afternoon Parallel Session***		
	Analytical Sciences	[AS-021] … [AS-028]	CE 5
	Catalysis Science & Engineering	[CE-020], [CE-022], [CE-024] … [CE-028]	CE 2
	Computational Chemistry	[CC-021] … [CC-028]	CE 105
	Inorganic & Coordination Chemistry	[IC-021] … [IC-028]	CE 3
	Medicinal Chemistry & Chemical Biology	[MC-021] … [MC-028]	CE 6
	Organic Chemistry	[OC-021] … [OC-028]	CE 1
	Physical Chemistry	[PC-021] … [PC-028]	CE 4
	Polymers, Colloids & Interfaces	[PCI-021], [PCI-022], [PCI-024] … [PCI-028]	BS 160
	Exhibitor Apéro		CE
17.00	Break and coffee/refreshments		CE
17.15	KGF-SCS Distinguished Industrial Science Award Lecture 2015 [PS-003] Dr. ***Jürg Zimmermann,*** Novartis Pharma AG «Evolution in Medicinal Chemistry»		CE 6
18.00	Best Oral Presentation Awards (sponsored by Metrohm) Presented by Dr. Markus Tobler, CEO Metrohm Schweiz AG		CE 6
18.15	Best Poster Presentation Awards (sponsored by DSM) Presented by Dr. Thomas Netscher, principal scientist at DSM		CE 6
18.30	End of the conference		

GENERAL INFORMATION

Date: September 4, 2015, 09.00–18.30
Location: École Polytechnique Fédérale de Lausanne EPFL
CE and BS Building
CH-1015 Lausanne

Chair and local Organizer

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Organizing Committee

Chairpersons
– Prof. Sandrine Gerber, EPF Lausanne (Chair)
– Prof. Christian Bochet, University of Fribourg (co-Chair)

Analytical Sciences
– Dr. Stefan Schürch, University of Bern
– Dr. Hanspeter Andres, Federal Institute of Metrology METAS

Catalysis Science and Engineering
– Prof. Paul Dyson, EPF Lausanne
– Prof. Kevin Sivula, EPF Lausanne

Computational Chemistry
– Prof. Clémence Corminboeuf, EPF Lausanne
– Prof. Tomasz Wesolowski, University of Geneva

Inorganic Chemistry
– Prof. Kay Severin, EPF Lausanne
– Prof. Lothar Helm, EPF Lausanne

Medicinal Chemistry and Chemical Biology
– Dr. Yves Auberson, Novartis Pharma AG

Organic Chemistry
– Prof. Philippe Renaud, University of Bern
– Prof. Nicolas Winssinger, University of Geneva

Physical Chemistry
– Prof. Stefan Willitsch, University of Basel
– Prof. Fréderic Merkt, ETH Zurich

Polymers, Colloids and Interfaces
– Prof. Holger Frauenrath, EPF Lausanne
– Prof. Markus Niederberger, ETH Zurich

Admission

Presenters (Poster and/or Talk)
– SCS Members: free of charge (she/he, whose name is underlined in the abstract)
– Non-members: CHF 250

Participants
– SCS Members: free of charge
– Non-members: CHF 50. Pre-registered participants will receive an invoice in advance to avoid waiting at the check-in desk. Pre-registration is possible until August 20, 2015.

If attending as a SCS member you must bring your SCS membership-card with you!

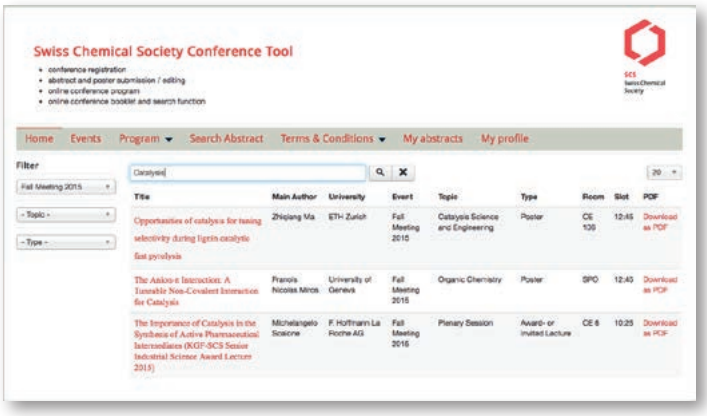
Pre-registration as participant on *http://chemistrycongresses.ch* is possible until Aug 20, 2015.

SCS Membership

A SCS membership offers many benefits. For information please see the SCS webpage. To join the society you can register via the online form. *http://scg.ch/membership/*
After registration as a member, your login data can also be used for the SCS Conference Tool.

Conference Tool

The conference tool provides a wide range of new functionalities and offers an easy and interactive planning of your conference day.
Go to ***http://chemistrycongresses.ch***, login with your SCS login 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 users mailbox
– Extensive search functionality



Coffee Breaks and Lunch

Complementary refreshments will be served before the opening ceremony and during the breaks. Lunch sandwiches and drinks will be served during the lunch break.
There is the 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) offers you access to the internet. Members of institutions participating to the Switch-Mobile project (all Swiss universities) will be able to connect by simply using their usual VPN client software. Other users will have to register first through a secure web page or can use the Swisscom Hotspot.

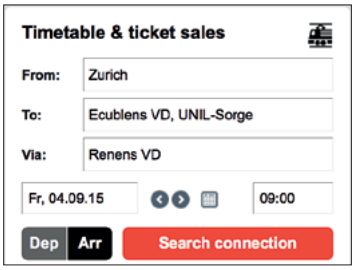
Conference Venue at EPFL Lausanne

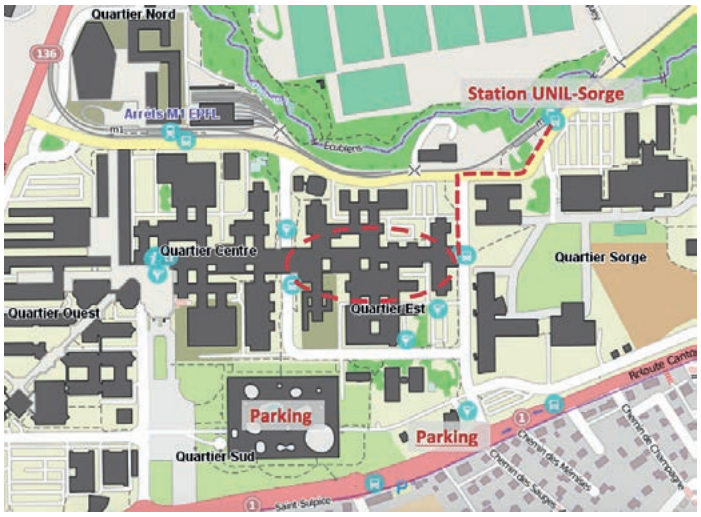
Conference Location

The meeting will be held on the first floor of the BS and CE buildings. Participants are kindly requested to use exclusively the East entrance on the first floor of BS building. The nearest tramway station is UNIL-Sorge (upper-right corner on the map). The way from the tramway station and from the parking lot to the entrance of the conference premises will be marked out with signs.

Transportation

By train: the easiest way to access the location by public transportation is via Renens, VD. Go to *www.sbb.ch* and select *Ecublens VD, UNIL-Sorge* via *Renens VD* as destination:



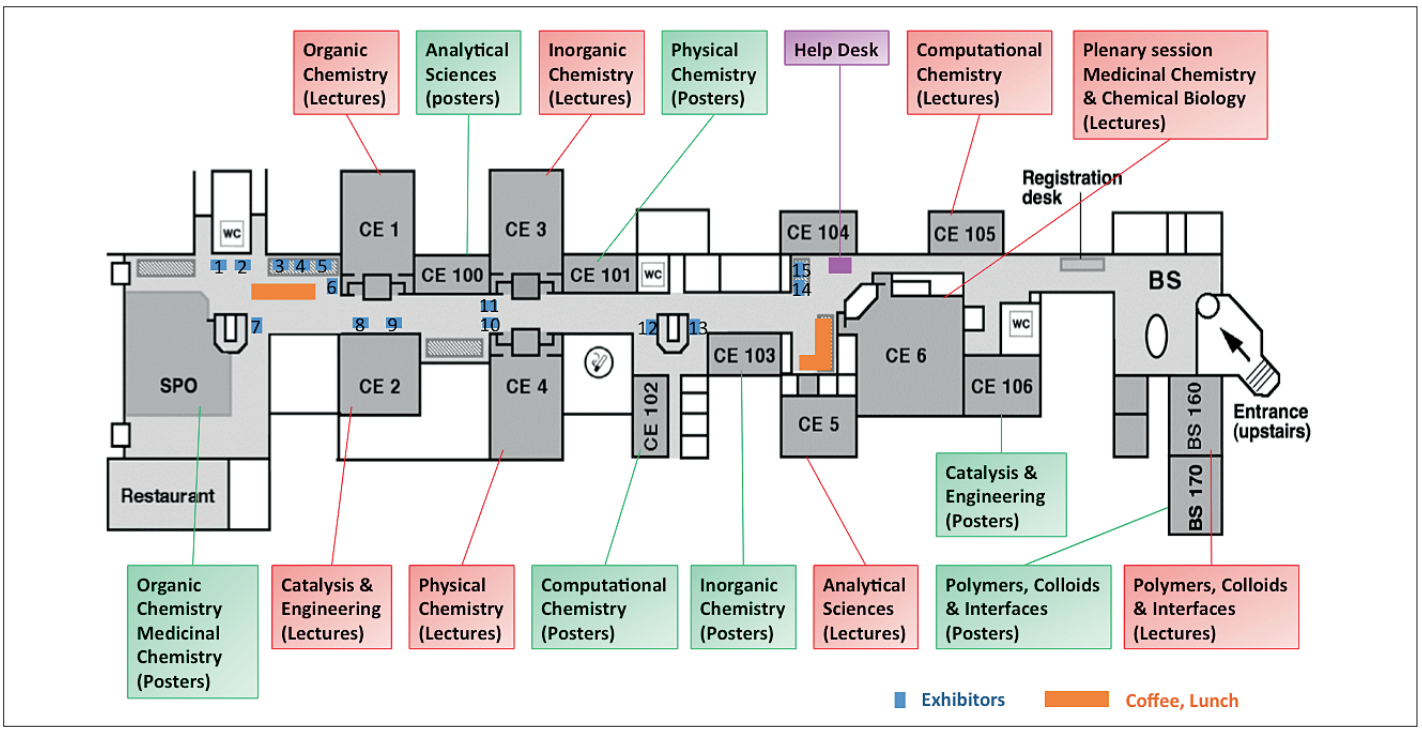


More information on how to get to EPFL campus, timetables and interactive maps are available on the webpage at *http://map.epfl.ch*.

By car: on the motorway, follow Lausanne-Sud, exit at UNIL-EPFL, drive West for 1.7 km and then turn right at the sign EPFL. Limited space will be available at the parking of the building Odyssea and of the Rolex Learning Center (see EPFL campus map). One-day parking permits will be sold on the parking lot and at the entrance of the BS building for CHF 5.

Site map, CE and BS Buildings

Session	Lectures	Posters
Opening Ceremony, Plenary Sessions	CE 6	
Analytical Sciences	CE 5	CE 100
Catalysis Science & Engineering	CE 2	CE 106
Computational Chemistry	CE 105	CE 102
Inorganic & Coordination Chemistry	CE 3	CE 103
Medicinal Chemistry & Chemical Biology	CE 6	SPO
Organic Chemistry	CE 1	SPO
Physical Chemistry	CE 4	CE 101
Polymers, Colloids & Interfaces	BS 160	BS 170



Main Sponsors

Main 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.

Presentation Awards 2015

Best Oral Presentation Award

The prize is given for the best presentations in 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 plenary lecture hall CE 6.

Prizes for Winners
- 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 Runners' up
Cash contribution of CHF 400.

The prize is sponsored by Metrohm.

Winners Best Oral Presentation Award 2014, SCS Fall Meeting 2014, University of Zurich

Best Poster Presentation Award

The prizes are given for the best posters in 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 plenary lecture hall CE 6.

Prizes for Winners
- Cash contribution of CHF 500.
- Travel voucher of CHF 750 to attend an international conference.
- Invitation to present the research in the laureates' issue of CHIMIA. Value CHF 1'200.

Prizes for Runners' up
- Cash contribution of CHF 300.

The prize is sponsored by DSM.

Winners Best Poster Presentation Award 2014, SCS Fall Meeting 2014, University of Zurich

معهد قطر لبحوث
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Qatar Environment & Energy
Research Institute
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About QEERI

Qatar Environment and Energy Research Institute (QEERI) is a member of Qatar Foundation for Education, Science and Community Development and is under the umbrella of Hamad Bin Khalifa University. As a national research institute, QEERI plays a leading role addressing the national Energy and Water Security Grand Challenges through Research and Development (R&D).

Aligned with the Qatar National Vision 2030's strategy of transforming the State into a diverse and sustainable knowledge-based economy, QEERI's water R&D program is developing innovative technologies in water desalination and treatment; water quality and reuse; aquifer recharge; climate change and atmospheric science; and water conservation. QEERI's energy R&D focuses on solar Photovoltaics (PV), energy storage, grid integration and energy efficiency.

www.qeeri.org.qa

SESSION ENDOWMENTS

Plenary Session

EPF Lausanne, School of Basic Sciences
The School of Basic Sciences is responsible for teaching and research in chemistry, mathematics, physics and related domains. A growing emphasis has been developing in fields at the interface between traditional disciplines, both within and outside of our School. Our interaction with the School of Life Sciences is particularly strong, as evidenced by jointly appointed professors, collaborative projects and shared infrastructure. To carry out our mission, we possess state-of-the art research facilities, support services and infrastructure.
[http://sb.epfl.ch]

Catalysis Sciences & Engineering Session

Clariant International Ltd
Clariant, a world leader in specialty chemicals, employed a total workforce of 17,003 in 60 countries and recorded sales of CHF 6.116 billion in 2014. Based on the four Business Areas Care Chemicals, Catalysis, Natural Resources, and Plastics & Coatings Clariant contributes to value creation with innovative and sustainable product solutions for its customers. Our research and development activities do not only focus on specific customer needs but also address the key trends of our time such as resource and energy efficiency or renewable raw materials.
[www.clariant.com]

Inorganic & Coordination Chemistry Session

Contact Group for Research Matters (KGF)
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]

Medicinal Chemistry & Chemical Biology Session

Actelion Ltd
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]

Organic Chemistry Session

Syngenta Crop Protection AG
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]

Physical Chemistry Session

Bruker BioSpin
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]

Polymers, Colloids & Interfaces

Dow Europe GmbH
Dow (NYSE: 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]

Commercial Exhibition

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 CE building, right in front of the lecture halls and the coffee and lunch desks.

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http://www.advion.com

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http://www.agilent.ch

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EQUILABO
Fournisseur de réacteurs et de calorimètres
http://www.equilabo.com

IG Instruments
smart solutions & service
http://igz.ch

LOT
QuantumDesign
http://www.lot-qd.de

MERCK MILLIPORE
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Metrohm
Schweiz AG
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Award Lectures Overview

09:55 ***Stefan Abele***, ***Jacques-Alexis Funel*** and ***Gunther Schmidt*** from Actelion Pharmaceuticals Ltd, ***Roger Marti***, Hochschule für Technik und Architektur Fribourg, ***Christian Mössner***, ***Mischa Schwaninger***, Swissi Process Safety, a member of TÜV SÜD Groupis, are awarded the Sandmeyer Award 2015 for the conception and successful scale-up of Diels–Alder reactions and organocatalysis leading to enantiomerically pure 5-phenylbicyclo[2.2.2]oct-5-en-2-one, a key intermediate for the production of an L/T calcium channel antagonist.

Stefan Abele will give the award lecture with the title «**Daring the Challenge and Thinking Big: the Value of Early Process Research**» [PS-001] ; Lecture hall CE 6.

10:25 ***Michelangelo Scalone***, F. Hoffmann La Roche, is awarded the KGF-SCS Senior Industrial Science Award 2015 for his outstanding contributions to the design of new, short and cost-efficient syntheses for many development projects by applying asymmetric catalytic reactions, and for his longtime success and expertise in leading the Center of Excellence Catalysis at Roche.

«**The Importance of Catalysis in the Synthesis of Active Pharmaceutical Intermediates**» [PS-002] ; Lecture hall CE 6.

11:15 ***Prof. Natalie Banerji***, University of Fribourg, is awarded the Grammaticakis-Neumann Award 2015 for her research combining synthesis, photochemistry, photophysics, and molecular photobiology to develop artificial photo-synthesis.

«**Unraveling the Photophysical Properties of Organic Semiconductors**» [PC-011]; Lecture hall CE 4.

11:30 ***Dietmar Hüglin***, BASF Schweiz AG, is awarded the KGF-SCS Industrial Science Award 2015 for his contribution in developing new ingredients for consumer product markets and specifically for the discovery, research & development of cosmetic UV absorbers combining chemistry with nano-technology. These innovations are setting currently the global standards in high performance photo-protection of human skin.

«**New UV Absorbers for the Photo-protection of Human Skin**» [PCI-012] ; Lecture hall BS 160.

17:15 ***Jürg Zimmermann***, Novartis Pharma AG, is awarded the KGF-SCS Distinguished Industrial Science Award 2015 for the ground breaking discovery of protein kinase inhibitors, which had a tremendous impact on the research and therapy of cancer and other diseases. The discovery and development of Imatinib (Gleevec) has revolutionized the therapy of certain forms of leukemia, and also had a tremendous impact on research projects both in industry and academia.

«Evolution in Medicinal Chemistry»
[PS-003] ; Lecture hall CE 6.

Plenary Sessions – CE 6

Chair: Prof. Dr. E. Peter Kündig

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Session Endowment: EPFL, School of Basic Sciences

09:55 **Daring the Challenge and Thinking Big: the Value of Early Process Research (Sandmeyer Award Lecture 2015) [PS-001]**
Stefan Abele, Actelion Pharmaceuticals Ltd.

10:25 **The Importance of Catalysis in the Synthesis of Active Pharmaceutical Intermediates (KGF-SCS Senior Industrial Science Award Lecture 2015) [PS-002]**
Michelangelo Scalone, F. Hoffmann La Roche AG

17:15 **Evolution in Medicinal Chemistry (KGF-SCS Distinguished Industrial Science Award Lecture 2015) [PS-003]**
Jürg Zimmermann, Novartis Pharma AG

Abstract codes

[XY-001]...[XY-009]	Award lectures, plenary sessions
[XY-010]...[XY-019]	Morning session lectures
[XY-020]...[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
PCI	Polymers Colloids & Interfaces
PS	Plenary Session

Name (regular font) = Presenting Author
Name (italic font) = Research Leader

Parallel Sessions

Analytical Sciences [AS]
Morning Session – CE 5
Chair: Hanspeter Andres, METAS

No session endowment

11:15 **MIR Spectroscopy beyond trace levels - environmental and industrial applications [AS-011]**
Lukas Emmenegger, EMPA Dübendorf

12:00 **Detection and identification of non-covalent interactions with SPRi-MALDI MS [AS-014]**
Ulrike Anders, *Renato Zenobi*, ETH Zurich

12:15 **Quick and easy NMR titration using slice-selective experiments to study concentration gradients in agarose gels [AS-015]**
Yavor Mitrev, *Damien Jeannerat*, University of Geneva

12:30 **High-speed, high-resolution, multi-elemental imaging of geological samples [AS-016]**
Marcel Burger, *Detlef Günther*, ETH Zurich

Afternoon Session – CE 5
Chair: Stefan Schürch, University of Bern

15:00 **Electromembrane extraction: a new technical development. [AS-021]**
Nicolas Drouin, *Julie Schappler*, University of Geneva

15:15 **Drug quantification in blood within microstructures for Point-of-Care Therapeutic Drug Monitoring [AS-022]**
Elena-Diana Burghelea, *Jean-Manuel Segura*, HES-SO Valais

15:30 **Thin Layer Ionophore-Based Membranes for Multianalyte Detection [AS-023]**
Maria Cuartero, University of Geneva

15:45 **Multistage Transversal Modulation Ion Mobility Spectrometry: Reducing the Voltage Required for High Resolution IMS for pre-existing mass spectrometers. [AS-024]**
Miriam Macia, SEADM S.L., *Guillermo Vidal-de-Miguel*, ETH Zurich

16:00 **Fourier optical beam shaping of femtosecond laser pulses for high resolution depth profile analyses by LA-ICPMS [AS-025]**
Debora Käser, *Detlef Günther*, ETH Zurich

16:15 **High resolution laser ablation depth-profiling mass spectrometry [AS-026]**
Andreas Riedo, *Peter Wurz*, University of Bern

16:30 **Single-walled Carbon Nanotubes (SWCNTs) for Bioanalyte Sensing [AS-027]**
Justyna Kupis-Rozmyslowicz, *Ardemis Anoush Boghossian*, EPF Lausanne

16:45 **Variable Q1 windows for MS acquisition and predicted LC retention time ranges for LC-SWATH-MS analysis [AS-028]**
Tobias Bruderer, *Gérard Hopfgartner*, University of Geneva

Computational Chemistry [CC]
Morning Session – CE 105
Chair: Tomasz Wesolowski, University of Geneva

Session endowment: QEERI

11:15 **Challenges of Electronic Structure Calculations: Hamiltonian Gadgets with Reduced Resource Requirements [CC-011]**
Sabre Kais, Qatar Environment and Energy Research Institute, Doha, Qatar

11:45 **Addressing the selection bias: Genetically optimized molecular data sets to train machine learning models of atomization enthalpies [CC-013]**
Nicholas Browning, *Ursula Röthlisberger*, EPF Lausanne

12:00 **Tunneling and Parity Violation in Trisulfane (HSSSH): An Almost Ideal Molecule for Detecting Parity Violation in Chiral Molecules [CC-014]**
Csaba Fabri, *Martin Quack*, ETH Zurich

12:15 **Molecular Dynamics with inter-system crossing and nonadiabatic effects [CC-015]**
Felipe Franco de Carvalho, EPF Lausanne/CECAM

12:30 **Local density fitting within a Gaussian and plane waves approach [CC-016]**
Dorothea Golze, *Jürg Hutter*, University of Zurich

Afternoon Session – CE 105
Chair: Jiri Vanicek, EPF Lausanne

15:00 **Interactive Similarity Maps for Visualization of High Dimensional Chemical Spaces [CC-021]**
Mahendra Awale, *Jean-Louis Reymond*, University of Bern

15:15 **Addressing the Rare Event Sampling problem with the PINS and SA-MC Methods : studying Structure and Dynamics of the Myoglobin protein [CC-022]**
Florent Hédin, *Markus Meuwly*, University of Basel

15:30 **Accelerating Quantum Instanton Calculations of Kinetic Isotope Effects [CC-023]**
Konstantin Karandashev, *Jiri Vanicek*, EPF Lausanne

15:45 **First principles based crystal structure prediction from alchemical coupling [CC-024]**
Alisa Solovyeva, University of Basel

16:00 **Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry [CC-025]**
Riccardo Petraglia, *Clemence Corminboeuf*, EPF Lausanne

16:15 **Interface effects in the case of dry reforming – CO_2 activation on Ni-supported γ-Al_2O_3 and Ni-nanoparticles vs ideal Ni(111) surface [CC-026]**
Marius-Christian Silaghi, *Christophe Copéret*, ETH Zurich

16:30 **Response time of quantum-chemical calculations during real-time reactivity explorations [CC-027]**
Alain C. Vaucher, *Markus Reiher*, ETH Zurich

16:45 **Orthogonality of embedded wave functions for different states in Frozen-Density Embedding Theory [CC-028]**
Alexander Zech, *Tomasz Adam Wesolowski*, University of Geneva

Catalysis Sciences & Engineering [CE]
Morning Session – CE 2

Chair: Kevin Sivula, EPF Lausanne

Session Endowment: Clariant International Ltd

11:15 **Reversible Electrocatalysis by Enzymes of Relevance to Renewable Energy Conversions [CE-011]**
Fraser Armstrong, University of Oxford

11:45 **Earth-abundant Electrocatalysts for Solar Fuels Production [CE-013]**
Carlos G. Morales-Guio, *Xile Hu*, EPF Lausanne

12:00 **Halogen chemistry on rutile-type catalysts [CE-014]**
Maximilian Moser, *Javier Pérez-Ramírez*, ETH Zurich

12:15 **Intermediates in the Photochemical Dehydrogenation of Borane-Amines [CE-015]**
Muhammad Sohail, Qatar Environment & Energy Research Institute (QEERI)

12:30 **Challenges in photocatalytic water reduction with nickel containing polyoxometalates [CE-016]**
René Moré, *Greta Ricarda Patzke*, University of Zurich

Afternoon Session – CE 2

Chair: Javier Pérez-Ramírez, ETH Zurich

14:45 **Development of MTPROP® catalysts: Basis for the realisation of the Methanol-To-Propylene process [CE-020]**
Markus Tonigold, Clariant AG

15:15 **Synthetic Chemistry to Reduce CO_2 Emissions [CE-022]**
Matthew Kanan, Stanford University

15:45 **Incorporation of ruthenium catalytic centers in phosphine-functionalized metal-organic frameworks [CE-024]**
Flavien Lucas Morel, ETH Zurich, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

16:00 **NMR Signatures of the Active Sites in Sn-β Zeolite [CE-025]**
Aleix Comas-Vives, *Christophe Copéret*, ETH Zurich

16:15 **Active and spectator Ce^{3+} species in a ceria-based platinum catalyst during low-temperature CO oxidation [CE-026]**
René Kopelent, *Olga V. Safonova*, Paul Scherrer Institute, Villigen

16:30 **Generation of NH_3-SCR active catalysts from decomposition of supported $FeVO_4$ [CE-027]**
Adrian Marberger, Paul Scherrer Institut, *Oliver Kröcher, Paul Scherrer Institute, Villigen and EPF Lausanne*

16:45 **Direct conversion of cellulose into HMF [CE-028]**
Sviatlana Siankevich, *Paul Dyson*, EPF Lausanne

Inorganic & Coordination Chemistry [IC]
Morning Session – CE 3

Chair: Kay Severin, EPF Lausanne

Session Endowment: Contact Group for Research Matters (KGF)

11:15 **The Magic of Polypnictogen-based Chemistry [IC-011]**
Manfred Scheer, Universität Regensburg

12:00 **Chemoselective Alkene Hydrosilylation Catalyzed by Nickel Pincer Complexes [IC-014]**
Ivan Buslov, *Xile Hu*, EPF Lausanne

12:15 **Chiral $(NH)_2P_2$ Macrocyclic Iron(II) Complexes: Design and Application in the Highly Enantioselective Transfer Hydrogenation of Ketones [IC-015]**
Raphael Bigler, *Antonio Mezzetti*, ETH Zurich

12:30 **Cobalt Complexes of Tetradentate, Bipyridine-Based Macrocycles for Highly Active Hydrogen Evolution in Aqueous Photocatalysis [IC-016]**
Evelyne Joliat, *Roger Alberto*, University of Zurich

Afternoon Session – CE 3

Chair: Marinella Mazzanti, EPF Lausanne

15:00 **Two Synthetic Approaches for one target: Single Molecule Magnet Behaviour [IC-021]**
Pierre Emmanuel Car, University of Zurich

15:15 **Self-assembly of 3d-5f Molecular Magnets from Pentavalent Uranyl [IC-022]**
Lucile Chatelain, *Marinella Mazzanti*, EPF Lausanne

15:30 **On the Synthesis, Biological Evaluation and Use of Metallocenyl Derivatives [IC-023]**
Jeannine Hess, *Gilles Gasser*, University of Zurich

15:45 **Vibrational spectroscopy on functionalized and chiral monolayer protected gold clusters [IC-024]**
Birte Varnholt, *Thomas Bürgi*, University of Geneva

16:00 **Carbene insertion into a P–H bond: Parent phosphinidene-carbene adducts from PH_3 [IC-025]**
Mark Bispinghoff, *Hansjörg Grützmacher*, ETH Zurich

16:15 **Design and Synthesis of Perfluorous Ionic Liquids [IC-026]**
Valentin Michael Manzanares, *Paul Joseph Dyson*, EPF Lausanne

16:30 **Going to Extremes: From Fluorine-Free Blue to Stable Red Emitting Iridium Complexes for LEECs [IC-027]**
Cathrin D. Ertl, *Edwin C. Constable*, University of Basel

16:45 **Application of ferrocene derivatives for stimuli-responsive polymers and for biosensor [IC-028]**
Michela Di Giannantonio, *Katharina Fromm,* University of Fribourg

Medicinal Chemistry & Chemical Biology [MC]
Morning Session – CE 6

Chair: Yves Auberson, Novartis

Session Endowment: Actelion Ltd

11:15 **SCS Division of Medicinal Chemistry: What does the DMCCB do? [MC-011]**
Yves Auberson, Novartis Pharma AG

11:30 **Discovery and optimisation of a CREBBP Bromodomain ligand. [MC-012]**
Michael Brand, *Robert S. Paton*, University of Oxford

11:45 **LC-MS/MS for determination of brain uptake and target mediated differential PK of PDE10A PET tracer candidates [MC-013]**
Gobbi Luca, F. Hoffmann-La Roche AG

12:00 **Synthetic Nucleotides Reduce Human DNA Polymerase η-mediated Synthesis Over a Cisplatin DNA Cross-link Adduct [MC-014]**
Arman Nilforoushan, *Shana Sturla*, ETH Zurich

12:15 **Discovery of G Protein-Coupled Bile Acid Receptor 1 (GPBAR1, TGR5) Agonists as Antiinflammatory Agents [MC-015]**
Klemens Hoegenauer, Novartis Pharma AG

12:30 **From pre-miRNA labeling to the identification of small molecule modulators of microRNA biogenesis: application to the cancer associated pre-let-7/lin28 interaction. [MC-016]**
Ugo Pradere, *Jonathan Hall*, ETH Zurich

Afternoon Session – CE 6

Chair: Jean-Louis Reymond, University of Bern

15:00 **Fluoroquinolone containing inhibitors of bacterial topoisomerases with a novel mode of action [MC-021]**
Cornelia Zumbrunn, Actelion Pharmaceuticals Ltd.

15:15 **Siglec-8 – A Novel target For Asthma. [MC-022]**
Blijke Suzanne Kroezen, *Beat Ernst*, University of Basel

15:30 **SMN2 splicing modifier for the treatment of Spinal Muscular Atrophy (SMA) [MC-023]**
Hasane Ratni, F. Hoffmann-La Roche AG

15:45 **From bulk to single molecule - Point mutations reveal specific intra domain interactions essential for group II intron ribozyme folding [MC-024]**
Erica Fiorini, *Roland K.O. Sigel*, University of Zurich

16:00 **Photoaffinity labeling in Chemoproteomic: Cyanopindolol and a small molecule mediated reprogramming of mESCs as successful case study. [MC-025]**
Maude Patoor, *Laure C. Bouchez*, Novartis Pharma AG

16:15 **Refining the understanding of the catalytic mechanism of DNAzymes [MC-026]**
Marcel Hollenstein, University of Bern

16:30 **Strigolactones and their potential role in modern agriculture [MC-027]**
Mathilde Lachia, Syngenta Crop Protection AG

16:45 **Guineensine as a Novel Inhibitor of Endocannabinoid Reuptake [MC-028]**
Ruben Bartholomäus, ETH Zurich, *Jürg Gertsch, University of Bern*

Organic Chemistry [OC]
Morning Session – CE 1

Chair: Nicolas Winssinger, University of Geneva

Session Endowment: Syngenta Crop Protection AG

11:15 **Total Synthesis of Mandelalide A [OC-011]**
Tobias Brütsch, *Karl-Heinz Altmann*, ETH Zurich

11:30 **First Enantioselective Total Synthesis of Terengganensine A [OC-012]**
Cyril Piemontesi, *Jieping Zhu*, EPF Lausanne

11:45 **Synthesis of Cyclopentenones by an Asymmetric Nickel-Catalyzed [3+2] Reductive Cycloaddition of Enoates with Alkynes [OC-013]**
Joachim Ahlin, *Nicolai Cramer*, EPF Lausanne

12:00 **Catalytic One-Step Synthesis of Unprotected Piperazines, Morpholines and Thiomorpholines using SnAP Reagents [OC-014]**
Michael U. Luescher, *Jeffrey W. Bode*, ETH Zurich

12:15 **Organocatalytic Atroposelective Aldol Condensation [OC-015]**
Achim Link, University of Basel, *Christof Sparr*, ETH Zurich

12:30 **Lewis Acid Catalyzed Electrophilic Trifluoromethylation of Silyl Ketene Acetals: Access to Quaternary α-Trifluoromethylated Esters and Lactones [OC-016]**
Dmitry Katayev, *Antonio Togni*, ETH Zurich

Afternoon Session – CE 1

Chair: Philippe Renaud, University of Bern

15:00 **DAST-mediated Cyclization of a,a-Disubstituted-a-acylaminoketones: Efficient and Divergent Synthesis of Unprecedented Heterocycles [OC-021]**
Aurelien Bigot, Syngenta Crop Protection AG

15:15 **Design, synthesis and properties of 'Photochomic Torsional Switches' (PTS) [OC-022]**
Giuseppe Sforazzini, EPF Lausanne

15:30 **Dancing Ladders - Inducing and Distorting Helical Chirality in Achiral Polycyclic Systems [OC-023]**
Michel Rickhaus, *Marcel Mayor*, University of Basel

15:45 **Access to dihydrofurans with a fully substituted C2 stereocenter by Pd-catalyzed intermolecular asymmetric Heck reaction [OC-024]**
Gustavo Manuel Borrajo-Calleja, *Clement Mazet*, University of Geneva

16:00 **Domino Reaction to Functionalize Heterocycles: A Complementary Method to C-H Functionalization [OC-025]**
Yifan Li, *Jérôme Waser*, EPF Lausanne

16:15 **Pyridylidene-Mediated Dihydrogen Activation Coupled with Catalytic Imine Reduction [OC-026]**
Johanna Auth, *Andreas Pfaltz*, University of Basel

16:30 **Disclosing a Novel Way for Poly(disulfide)s to Enter Cells [OC-027]**
Giulio Gasparini, *Stefan Matile*, University of Geneva

16:45 **Halogen Bonding Supramolecular Capsules [OC-028]**
Oliver Dumele, *Franois Diederich*, ETH Zurich

Physical Chemistry [PC]

Morning Session – CE 4
Chair: Frédéric Merkt, ETH Zurich

Session Sponsoring: Bruker Physik GmbH

11:15 **Unraveling the Photophysical Properties of Organic Semiconductors (Grammaticakis-Neumann Award Lecture 2015) [PC-011]**
Natalie Banerji, University of Fribourg

11:45 **Kinetic Isotope Effects on Exchange Rates of H^N and D^N in Tryptophan [PC-013]**
Estel Canet, *Geoffrey Bodenhausen*, EPF Lausanne

12:00 **Photoinduced Stark effect in colloidal systems: a case study with $MAPbBr_3$ and AQU/nC_{60} [PC-014]**
Marine Eva Fedora Bouduban, *Jacques-E. Moser*, EPF Lausanne

12:15 **High resolution infrared spectroscopy and theory of parity violation and tunneling for dithiine as a candidate for measuring the parity violating energy difference between enantiomers of chiral molecules [PC-015]**
Sieghard Albert, *Martin Quack*, ETH Zurich

12:30 **Symmetry-Breaking Phenomena Detected with Ultrafast Time-Resolved Infrared Spectroscopy [PC-016]**
Bogdan Dereka, *Eric Vauthey*, University of Geneva

Afternoon Session – CE 4
Chair: Natalie Banerji, University of Fribourg

15:00 **Vibrational Optical Acitivity (VOA) of Chiral Ionic Liquids (CILs) [PC-021]**
Patric Oulevey, *Thomas Bürgi*, University of Geneva

15:15 **Characterization of Gd(III) chelators and combination of paramagnetic NMR with Gd(III)-nitroxide DEER in studies of biomacromolecules [PC-022]**
Luca Garbuio, *Maxim Yulikov*, ETH Zurich

15:30 **Experimental study of the ion-molecule reaction $H_2^+ + H_2 \rightarrow H_3^+ + H$ at low collision energies [PC-023]**
Pitt Allmendinger, *Frédéric Merkt*, ETH Zurich

15:45 **$ClHO_3S$ as a prototype system for studying photo-dissociation induced by OH stretching overtone excitation [PC-024]**
Sebastian Brickel, *Markus Meuwly*, University of Basel

16:00 **Cold Chemistry on a multi-functional ion trap chip [PC-025]**
Arezoo Mokhberi, *Stefan Willitsch*, University of Basel

16:15 **$(Benzonitrile)_2$ and $(meta\text{-}Cyanophenol)_2$: Influence of a Hydroxy Group on the Excitonic Splitting [PC-026]**
Franziska Balmer, *Samuel Leutwyler*, University of Bern

16:30 **Aqueous Catholyte for Rechargeable Li-O_2 and Li-Water Batteries [PC-027]**
Nam Hee Kwon, *Katharina M. Fromm*, University of Fribourg

16:45 **Quantifying Equilibrium Binding Affinity using 2D IR Spectroscopy and Non-native Amino Acids [PC-028]**
Klemens Lucas Koziol, *Peter Hamm*, University of Zurich

Polymers, Colloids & Interfaces [PCI]

Morning Session – BS 160
Chair: Holger Frauenrath, EPF Lausanne

Session Endowment: Dow Europe GmbH

11:00 **Dynamic bonds in fracture of soft materials [PCI-010]**
Costantino Creton, ESPCI ParisTech

11:30 **New UV Absorbers for the Photo-protection of Human Skin (Industrial Science Award Lecture 2015) [PCI-012]**
Dietmar Hüglin, BASF AG

12:00 **High dielectric permittivity elastomers for artificial muscles [PCI-014]**
Dorina Opris, EMPA Dübendorf

12:15 **Surface-initiated controlled radical polymerization from cellulose nanomaterials [PCI-015]**
Justin Zoppe, *Harm-Anton Klok*, EPF Lausanne

12:30 **High molecular weight poly(m,p-phenylene)s derived by Suzuki polycondensation: synthesis, processing and testing [PCI-016]**
Bernd Deffner, A. *Dieter Schlüter,* ETH Zurich

12:45 **Functionalized polymersomes inhibit malaria parasite invasion into host red blood cells [PCI-017]**
Adrian Najer, University of Basel

Afternoon Session – BS 160
Chair: Markus Niederberger, ETH Zurich

15:00 **Polyalkylene glycols and their role as components of modern industrial and automotive lubricants [PCI-021]**
Martin Greaves, Dow Europe GmbH, Dow Europe GmbH

15:15 **Droplet-Based Microfluidics: High-Throughput Experimentation One Drop at a Time [PCI-022]**
Andrew deMello, ETH Zürich

15:45 **Photo-Sensitive Cationic Nanocarriers for Non-Toxic Delivery of Small Molecules [PCI-024]**
Ionel Adrian Dinu, *Wolfgang Meier*, University of Basel

16:00 **From supramolecular sheets to fibers and back: establishing the critical parameters that govern the morphology of pyrene-based self-assembled materials [PCI-025]**
Mykhailo Vybornyi, *Robert Häner*, University of Bern

16:15 **Electron transfer through peptide assemblies [PCI-026]**
Sonja Kracht, *Katharina Fromm*, University of Fribourg

16:30 **Self-assembled 2-D WSe2 Thin Films for Photo-electrochemical Hydrogen production [PCI-027]**
Xiaoyun Yu, *Kevin Sivula*, EPF Lausanne

16:45 **Self-Recovering Gold Nanoparticle Films and Applications [PCI-028]**
Evgeny Smirnov, *Hubert Girault*, EPF Lausanne

Poster Sessions

Name (regular font) = Presenting Author
Name (italic font) = Main Research Leader

Analytical Sciences [AS]
Poster Session
Jury members: Stefan Schürch, University of Bern, Hanspeter Andres, METAS

Investigating the binding sites of RAPTA-C and RAPTA-EA to a 50 amino acid peptide using ETD fragmentation and ChemInfo algorithms [AS-101]
Laure Menin, *Paul Dyson,* EPF Lausanne,

Nano-SIMS to study the distribution of metal based anti-cancer compounds *in vitro* [AS-102]
Ronald FS Lee, *Paul Dyson,* EPF Lausanne

A Universal Low-Flow Secondary ElectroSpray Ionizer: High Sensitivity Volatile Analysis on Pre-existing MS Instruments [AS-103]
César Barrios, *Pablo Martinez-Lozano Sinues,* ETH Zurich

Characterization of a 2D Polymer Monolayer with Tip-Enhanced Raman Spectroscopy [AS-104]
Feng Shao, *Renato Zenobi,* ETH Zurich

Target plate material resistivity influences LDI efficiency [AS-105]
Guido Paul Zeegers, *Renato Zenobi,* ETH Zurich

Sr isotope ratios and Rb-Sr ages by LA-ICPMS with isobar separation by on-line electrothermal vaporization [AS-106]
Hale Ceren Yilmaz, *Bodo Hattendorf,* ETH Zurich

Full-metal AFM probes for tip-enhanced Raman spectroscopy [AS-107]
Jacek Szczerbiński, *Renato Zenobi,* ETH Zurich

MALDI-MS for Population Profiling with Single-Cell Resolution [AS-108]
Jasmin Krismer, *Renato Zenobi,* ETH Zurich

Observing gas-phase proton transfer reactions inside the MALDI plume [AS-109]
Mario Francesco Mirabelli, *Renato Zenobi,* ETH Zurich

Quantification of Trace Elements in Brass and Silicate Glasses by Portable Laser Ablation Sampling and Subsequent ICPMS [AS-110]
Peter Velicsanyi, *Detlef Günther,* ETH Zurich

Nucleoside phosphate monitoring in cell cultures using MALDI TOF MS [AS-111]
Robert Steinhoff, *Renato Zenobi,* ETH Zurich

Gap-mode TERS spectra of small organic amides and small peptides: is the amide I mode present? [AS-112]
Üzeyir Dogan, ETH Zürich

Novel fluorescence assays for monitoring recombinant proteins during biotechnological production and purification [AS-113]
Enrico Antonino Condemi, *Jean-Manuel Segura,* HES-SO Valais

Defensin Levels in Spider Hemolymph [AS-114]
Alena Krüger, *Stefan Schürch, University of Bern*

Binding of Metallocenes to Short Oligonucleotides [AS-115]
Rahel Eberle, *Stefan Schürch,* University of Bern

Elucidation of the gas-phase structure of a sugar-modified DNA analogue [AS-116]
Yvonne Hari, *Stefan Schürch,* University of Bern

Carbonate-Selective Potentiometric Solid Contact Electrode [AS-118]
Dajing J Yuan, *Eric Bakker,* University of Geneva

Efficient normal phase MS directed purification of natural products at the preparative scale [AS-119]
Davide Righi, *Jean-Luc Wolfender,* University of Geneva

Ion-selective Nanospheres as Heterogeneous Indicator Reagents in Complexometric Titrations [AS-120]
Jingying Zhai, *Eric Bakker,* University of Geneva

Charged Solvatochromic Dyes as Signal Transducers in Fluorescent and Colorimetric Ion Selective Nanosensors [AS-121]
Xiaojiang Xie, University of Geneva

Quantifying the detection capabilities of LA-ICPMS [AS-122]
Alex Ulianov, *François Bussy*, University of Lausanne

The ICPMS signal as a doubly stochastic Poisson process [AS-123]
Alex Ulianov, University of Lausanne

Online analysis of mass spectra of hydrocarbons [AS-124]
Luc Patiny, EPF Lausanne

Lipid droplets and large unilamellar lipid vesicles investigated by asymmetric-flow field-flow fractionation in combination with multi-angle light-scattering [AS-125]
Valerija Vezočnik, University of Ljubljana, *Ema Žagar, National Institute of Chemistry Slovenia*

Native nano-ESI-MS Applied to Fragment Based Drug Discovery [AS-126]
Agni Gavriilidou, *Renato Zanobi*, ETH Zurich

Unraveling the requirements for immortality – Phenotype characterization of the Δtlc1 Type II ALT survivors. [AS-127]
Alfredo J. Ibanez, ETH Zurich

UV-fs-LA-ICPMS of $La_{0.4}Ca_{0.6}MnO_3$ PLD thin Films [AS-128]
Kevin Guex, *Detlef Günther,* ETH Zurich

Dopant-induced conformational changes of proteins in the gas phase evaluated by Transversal Modulation Ion Mobility Spectrometry [AS-129]
Nicole Andrea Meyer, *Renato Zenobi,* ETH Zurich

Comprehensive detection of obstructive sleep apnea in humans and drug monitoring in mice by real-time breath analysis [AS-130]
Pablo Martinez-Lozano Sinues, ETH Zurich

Studying the 3-(2-Furoyl)quinoline-2-Carboxaldehyde (FQ) protein labelling reaction to improve accuracy of quantification in capillary electrophoresis-sodium dodecyl sulfate with laser induced fluorescence detection (CE-SDS-LIF) [AS-131]
Miriam Arrell, HES-SO Valais

Thin Layer Chemical Modulations by a Combined Selective Proton Pump and pH Probe for Direct Alkalinity Detection [AS-132]
Majid Ghahraman Afshar, *Eric Bakker,* University of Geneva

Ion-exchange nanosphere doped hydro-gel as buffer for electrochemical AS(III) detection in weakly buffered environmental media [AS-133]
Romain Touilloux, *Eric Bakker,* University of Geneva

Ion-selective fluorescent and pH independent nanosensors based on functionalized polyether macrocycles [AS-134]
Zdenka Jarolímová, *Eric Bakker*, University of Geneva

Solve complex and challenging mass spectrometry problems directly from the browser [AS-135]
Luc Patiny, EPF Lausanne

Chemical Composition and Biological Activities of Essential Oils Extracted from Pittosporum Mannii Hook (Pittosporaceae) [AS-136]
Souaibou Yaouba, University of Nairobi

Computational Chemistry [CC] Poster Session

Jury members: Tomasz Wesolowski, University of Geneva, Jiri Vanicek, EPF Lausanne, Matthew Wodrich, EPF Lausanne

Averaged Molecular Dynamics Trajectories in Frozen-Density Embedding Theory [CC-101]
Andrey Laktionov, EPF Lausanne, *Tomasz Adam Wesolowski, University of Geneva*

Effect of Mixed Organic Cations on the Phase Stability of Hybrid Organic/Inorganic Lead Perovskites for Solar Cell Applications [CC-102]
Ariadni Boziki, *Ursula Röthlisberger,* EPF Lausanne

Computational Investigations of a β-Class Carbonic Anhydrase from *Desulfovibrio vulgaris* [CC-103]
Esra Bozkurt, *Ursula Röthlisberger,* EPF Lausanne

Intramolecular symmetry-adapted perturbation theory - a tool for elucidating the weak intramolecular interactions [CC-104]
Ewa Pastorczak, *Jérôme Gonthier,* EPF Lausanne

Visualizing and quantifying molecular excited state interactions with scalar fields [CC-105]
Laurent Vannay, *Clemence Corminboeuf,* EPF Lausanne

Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B [CC-106]
Matej Repic, EPF Lausanne

A TD-DFT-based Approach to Describe Electron Dynamics of Molecules in Intense Laser Fields [CC-107]
Pablo Lopez Tarifa, *Ursula Röthlisberger,* EPF Lausanne

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-108]
Thibaud von Erlach, *Ursula Röthlisberger,* EPF Lausanne

Investigation of the Posttranslational Modifications Expressed in Polyteonamide B by Molecular Dynamics Simulations [CC-109]
Annick Renevey, *Sereina Riniker,* ETH Zurich

Mechanistic Study of Denitrification in Truncated Hemoglobin using Adiabatic Reactive Molecular Dynamics [CC-110]
Akshaya Kumar Das, University of Basel, *Markus Meuwly, University of Basel*

Assembly of a diverse 10M GDB Fragment Set [CC-111]
Ricardo Visini, *Jean-Louis Reymond,* University of Bern

DFT study of the influence of guest-host interactions on the high-spin/low-spin energy difference in $Co(bpy)_3^{2+}$@Y [CC-112]
Andrea Missana, *Andreas Hauser,* University of Geneva

Accounting for electronic polarization in subsystem DFT calculations [CC-113]
Emilie Chalaye-Chemineau, *Tomasz Adam Wesolowski,* University of Geneva

Study of Excited State Geometries of Organic Chromophores [CC-114]
Marie Humbert-Droz, University of Geneva

Pyrphyrin Adsorption on Au(111) Surface: Influence of Herringbone Reconstruction [CC-115]
Yeliz Gurdal, University of Zurich

Exploiting dispersion-driven aggregators as a route to new one-dimensional organic nanowires [CC-116]
Adrien Nicolai, *Clemence Corminboeuf,* EPF Lausanne

Statistical Averaging over Molecular Dynamics Ensembles in Frozen-Density Embedding Theory [CC-117]
Andrey Laktionov, EPF Lausanne, *Tomasz Adam Wesolowski, University of Geneva*

Molecular binding mechanism of a potent ruthenium-arene anticancer agent to the nucleosome core particle (NCP) [CC-118]
Giulia Palermo, *Ursula Röthlisberger,* EPF Lausanne

EVOLVE: a new genetic algorithm toolbox for protein engineering [CC-119]
Marta A. S. Perez, *Ursula Röthlisberger*, EPF Lausanne

The role of dispersion-correction in the description of metal-ligand bonds in density functional theory [CC-120]
Martin Peter Bircher, *Ursula Röthlisberger,* EPF Lausanne

The role of Mg^{2+} ions in adenylate cyclase [CC-121]
Siri Van Keulen, *Ursula Röthlisberger,* EPF Lausanne

The reactivity of hypervalent $\lambda^{3,4}$-iodanes explored using ab initio (meta-)dynamics [CC-122]
Oliver Sala, ETH Zurich

The new second-generation ETH DMRG program for quantum chemical applications [CC-123]
Stefan Knecht, *Markus Reiher,* ETH Zurich

Bohmian Mechanics with virtual particles [CC-124]
Oliver Thorsten Unke, *Markus Meuwly, University of Basel*

A Force Field Approach to Reproduce Grotthuss Mechanism in Reactive Systems [CC-125]
Zhen-Hao Xu, *Markus Meuwly,* University of Basel

New computational approaches for liquids and energy-related compounds [CC-126]
Sandra Luber, *Jürg Hutter,* University of Zurich

Physical Organic Characterisation of the Molecule-Electrode Contact in Single Molecule Junctions [CC-127]
Ganna Grynova, *Clemence Corminboeuf,* EPF Lausanne

Multicenter Bonding in Hypervalent λ^3-Iodanes: New Insight from the Analysis of Domain Averaged Fermi Holes [CC-128]
Halua Magalhães, ETH Zurich

Processing Data from Quantum Chemical Calculations using Turbomole-XML-eXist [CC-129]
Stefan Heinen, *Hans Peter Lüthi,* ETH Zurich

Thermal stability predictions as a tool for inherently safer process design [CC-130]
Nadia Baati, *Thierry Meyer,* EPF Lausanne

Catalysis Sciences & Engineering [CE] Poster Session

Jury members: S. David Tilley, University of Zurich, Jeremy Luterbacher, EPF Lausanne, Martin Albrect, University of Bern

Effect of the Pd-state in perovskite-type $A(B,Pd)O_{3\pm\delta}$ (A = La, Y; B = Mn, Fe, Co) oxidation catalysts in terms of CH_4-oxidation activity [CE-101]
Arnim Eyssler, EMPA Dübendorf

Hydrogen Storage in Formic Acid/Carbon Dioxide Systems - Solvent Effects: Heat of Mixing and pH of the Reaction Media [CE-102]
Cornel Fink, *Gábor Laurenczy,* EPF Lausanne

Insights into the Ionic Liquid-Promoted Electrochemical Reduction of CO_2 [CE-103]
Genevieve Lau, EPF Lausanne

Ni_2P nanoparticles as Janus catalyst for electrochemical water splitting [CE-104]
Lucas-Alexandre Stern, *Xile Hu,* EPF Lausanne

Aerogels for CO_2 Capture [CE-105]
Marco Roman Holzer, *Andreas Züttel,* EPFL Valais/Wallis

Selective dehydrogenation of formic acid over sub-nanometric gold particles supported on silica [CE-106]
Amaia Beloqui-Redondo, ETH Zürich

Esterification of 2-Methoxyphenol and Octanoic Acid over modified MCM-41 for Biomass Conversion [CE-107]
Bahir Duraki, ETH Zurich

Simple One-Pot Synthesis of Iridium-Titanium Oxide Composites [CE-108]
Emma Oakton, *Christophe Copéret,* ETH Zurich

Silver-indium catalysts for the electrochemical reduction of carbon dioxide [CE-109]
Gastón Larrazábal, *Javier Pérez-Ramírez,* ETH Zurich

Electrocatalysts for carbon dioxide recycling based on silver-indium materials [CE-110]
Gastón O. Larrazábal, *Javier Pérez-Ramírez,* ETH Zurich

Highly selective basic zeolites for the dehydrogenation of ethanol to acetaldehyde [CE-111]
Giacomo Marco Lari, *Javier Pérez-Ramírez,* ETH Zurich

Stability of tin-containing zeolites in continuous biomass conversions [CE-112]
Giacomo Marco Lari, *Javier Pérez-Ramírez,* ETH Zurich

Structure-performance relationships of hybrid nanocatalysts for selective hydrogenation [CE-113]
Gianvito Vilé, *Javier Pérez-Ramírez,* ETH Zurich

CO activation on Ruthenium Nanoparticles: *Ab Initio* calculations under reaction conditions. [CE-114]
Lucas Foppa, *Aleix Comas-Vives,* ETH Zurich

Impact of defect chemistry in zeolite desilication [CE-115]
Marilyne Boltz, *Javier Pérez-Ramírez,* ETH Zurich

Improving the Oxygen Evolution Kinetics of a Nanostructured Composite Hematite Photoanode [CE-116]
Mario Bärtsch, ETH Zurich, *Jan Augustyński, University of Warsaw*

Dehydrogenation and Polymerization on Cr(III) Silicates Are Rate-Determined by an Analoguous Mechanistic Step [CE-117]
Murielle F. Delley, *Christophe Copéret,* ETH Zurich

Improved Solution Finding in Industrial Waste Incineration Scheduling Through Implementation of Multi-Objective Strategies [CE-118]
Oliver Weder, *Konrad Hungerbühler,* ETH Zurich

Handling forecast uncertainty in industrial waste incineration scheduling [CE-119]
Ralph Bannerman, *Konrad Hungerbühler,* ETH Zurich

Towards a general pore connectivity index in hierarchically-organized zeolites by positron annihilation spectroscopy [CE-120]
Robbie Warringham, *Javier Pérez-Ramírez,* ETH Zurich

Integration of Hierarchical Waste Incineration Scheduling Levels for Improved Industrial Performance [CE-121]
Samuel Perren, *Konrad Hungerbühler,* ETH Zurich

Cu Particle Size and Support Effect on CO_2 Hydrogenation to MeOH over Supported Cu Catalysts [CE-122]
Shohei Tada, *Christophe Copéret,* ETH Zurich

Why does the addition of Fe increase the activity and stability of Ni-based dry reforming catalysts: An in-situ XRD and XAS study [CE-123]
Sung Min Kim, *Christophe Copéret,* ETH Zurich

Atomistic Description of Silica Supported (SiO)W(NAr)(=CHtBu)(OR) Catalysts Through DNP-SENS [CE-124]
Ta-Chung Ong, *Christophe Copéret*, ETH Zurich

Design of mild base catalysts for the deoxygenation of bio-oil by aldol condensation [CE-125]
Tobias Keller, *Javier Pérez-Ramírez,* ETH Zurich

Fast pyrolysis of lignin: Relating the Structure with Product selectivity [CE-126]
Victoria Custodis, *Jeroen A. van Bokhoven* ETH Zurich/PSI Villigen

Novel catalysts for the oxybromination of methane [CE-127]
Vladimir Paunovic, *Javier Pérez-Ramírez,* ETH Zurich

Encapsulated Polarizing Agents for Application in Dynamic Nuclear Polarization Surface Enhanced NMR Spectroscopy [CE-128]
Wei-Chih Liao, *Christophe Copéret,* ETH Zurich

Opportunities of catalysis for tuning selectivity during lignin catalytic fast pyrolysis [CE-129]
Zhiqiang Ma, *Jeroen A. van Bokhoven* ETH Zurich/PSI Villigen

Electrocatalytic water oxidation with $Co_{1-x}M_xNCN$ metal carbodiimides [CE-130]
Rafael Müller, *Greta Ricarda Patzke, University of Zurich*

Approaches towards heterogenization of Ru(II) half-sandwich catalysts for asymmetric hydrogenation [CE-131]
Beáta Vilhanová, Institute of Chemical Technology, Prague, Czech Republic, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

Hierarchical Pd/ZSM-5 catalysts for methane oxidation in the presence of steam [CE-132]
Andrey W. Petrov, *Jeroen A. van Bokhoven,* PSI Villigen

Structural analysis of individual Fluid Catalytic Cracking catalyst particle studied by synchrotron-based ptychographic X ray-computed tomography [CE-133]
Julio C. da Silva, PSI Villigen, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

Exploring the self-regenerating function of perovskit-type oxides on catalytically active nickel [CE-134]
Patrick Steiger, PSI Villigen

Time-resolved measurements of the terahertz conductivity in noble metal-on-TiO_2 nanoparticles for photocatalytic applications [CE-135]
Arno Schneider, PSI Villigen, *Jacques-E. Moser, EPF Lausanne*

Dual-phase Zn-modified ceria nanocrystals: establishing a correlation between the structural characteristics, oxygen storage capacities and catalytic activities [CE-136]
Fangjian Lin, PSI Villigen

From mechanism to catalyst design: Highly active formic acid decomposition catalysts under SCR-relevant conditions [CE-137]
Manasa Sridhar, PSI Villigen, *Oliver Kröcher, PSI Villigen and EPF Lausanne*

In situ X-ray Absorption Spectroscopy of $Ce_{0.5}Zr_{0.5}O_{2-d}$ at 1773 K [CE-138]
Matthäus Rothensteiner, PSI Villigen, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

Investigating the influence of CO and ceria on CH_4 abatement on Pd-based TWC using modulation excitation spectroscopy [CE-139]
Valentina Marchionni, PSI Villigen

Tuning reactant selectivity in the direct aldol-Tishchenko reaction using space constraints in multifunctional MOFs [CE-140]
Xiaoying Xu, PSI Villigen, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

Synthesis of hollow ZSM-5 nano-reactors containing copper-metal oxide nanoparticles [CE-141]
Jin Hee Lee, PSI, *Jeroen A. van Bokhoven, ETH Zurich/ PSI Villigen*

Engineering Streptavidin as Scaffold for the Design of Artificial Metalloenzymes [CE-142]
Hendrik Mallin, *Thomas R. Ward,* University of Basel

Towards cheap and sustainable energy sources by exploiting self-organized catalyst micro- and nano structures [CE-143]
Roche Marcel Walliser, *Edwin C. Constable,* University of Basel

Dynamic kinetic resolution of allylic acetates [CE-144]
Valentin Köhler, University of Basel

Heterogenization of chiral Ru(II) catalysts on mesoporous silica *via* the arene ligand [CE-145]
Jaroslav Aubrecht, University of chemistry and technology, *Petr Kačer, Institute of Chemical Technology, Prague, Czech Republic*

Synthesis of highly active ruthenium catalyst for transfer hydrogenation of ketones [CE-146]
Leoš Kořený, University of Chemistry and Technology, Prague, *Petr Kačer, Institute of Chemical Technology, Prague, Czech Republic*

TiO_2 and Ag-doped TiO_2 nanocontainers as photocatalysts for CO_2 reduction [CE-147]
Nelly Hérault, *Katharina Fromm,* University of Fribourg

Metal Center Tuning of Layered Double Hydroxides for Electrochemical Water Oxidation [CE-148]
Fabio Evangelisti, *Greta Ricarda Patzke,* University of Zurich

Doped Manganese Oxides as Water Oxidation Catalysts [CE-149]
Michael Olah, *Greta R. Patzke,* University of Zurich

Optimization of Ceria-Based Materials for Solar Thermochemical Two-Step CO_2-Splitting [CE-150]
Roger Jacot, University of Zurich, *Aldo Steinfeld, ETH Zurich*

Screening of Lewis Acidic Chlorometallate Ionic Liquids Combined with Nanoparticle Catalysts for Aromatic Hydrogenation Activity [CE-151]
Alena Karakulina, *Paul Joseph Dyson,* EPF Lausanne

Continuous flow synthesis of metal-organic frameworks utilizing microwave irradiation [CE-152]
Daniel Antti Steitz, ETH Zürich, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

Cationic co-doped TiO_2 nanoparticles as efficient visible-light active photocatalyst: experimental and theoretical study [CE-153]
Darinka Primc, ETH Zürich

Design and technical development of iron zeolite catalysts for the gas phase oxidation of glycerol to dihydroxyacetone [CE-154]
Giacomo Marco Lari, *Javier Pérez-Ramírez,* ETH Zurich

Zinc-rich copper catalysts promoted by gold for methanol synthesis [CE-155]
Oliver Martin, *Javier Pérez-Ramírez,* ETH Zurich

Evidence on the direct formation of methane from H_2O and CO_2 by thermochemical cycles using Ni- and Rh-doped ceria [CE-156]
Fangjian Lin, PSI Villigen

Towards stabilization of active methanation catalysts: Effect of boron promotion [CE-157]
Anastasios Kampolis, *Oliver Kröcher*, PSI Villigen

Superior durability of flame-made WO_3/CeO_x-TiO_2 $DeNO_x$ catalysts [CE-158]
Katarzyna Anna Michalow-Mauke, *Oliver Kröcher*, PSI Villigen

Photo-catalytic evolution of dihydrogen from water by Ni@MOF: a nickel catalyst encapsulated inside MIL-125-NH_2 (Ti) [CE-159]
Kim Meyer, PSI Villigen, *Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen*

Metal-support interaction of platinum nanoparticles supported on yttria stabilized zirconia catalysts for environmentally important reaction systems [CE-160]
Rima J Isaifan, Qatar Environment and Energy Research Institute (QEERI), *Elena A Baranova, University of Ottawa*

Inorganic Chemistry [IC] Poster Session

Jury members: Albert Ruggi, University of Fribourg, Gábor Laurenczy, EPF Lausanne, Anne-Sophie Chauvin, EPF Lausanne

Homogeneous Catalytic Hydrogen Storage and Release in the Formic Acid-Carbon Dioxide Couple using Ruthenium Pre-Catalysts [IC-101]
Antoine van Muyden, *Gábor Laurenczy,* EPF Lausanne

Self-sorting of Pd-based coordination cages: the importance of subtle steric effects [IC-102]
Giacomo Cecot, *Kay Severin,* EPF Lausanne

Small Molecule Activation at siloxide "ate" complexes of f elements [IC-103]
Julie Andrez, EPF Lausanne

A viable hydrogen storage and release system based on formate and bicarbonate salts: mechanistic insights into the hydrogen release step. [IC-104]
Katerina Sordakis, *Gábor Laurenczy,* EPF Lausanne

Multi-Electron Redox Reactions Promoted by f-Elements Complexes [IC-105]
Marta Falcone, *Marinella Mazzanti,* EPF Lausanne

Carboxylic acid-functionalized clathrochelate complexes as scaffolds for supramolecular metalloligands [IC-106]
Mathieu Marmier, *Kay Severin,* EPF Lausanne

Selective Hydrogen Production from Formic Acid: Development of Homogeneous Iron Catalysts in Aqueous Solution [IC-107]
Mickael Montandon-Clerc, *Gábor Laurenczy,* EPF Lausanne

Supramolecular cages from clathrochelates and stabilized imines [IC-108]
Suzanne Maria Jansze, *Kay Severin,* EPF Lausanne

Nickel Complexes as Catalysts for Silane Dehydrogenation and Hydrogenative Cleavage Reactions of Oligosilanes. [IC-109]
Bruno Pribanic, *Hansjörg Grützmacher,* ETH Zurich

Synthesis of New Polarization Matrices for Dynamic Nuclear Polarization [IC-110]
Daniel L. Silverio, *Christophe Copéret,* ETH Zurich

The Mechanism of C-H activation by Transition Metal Siloxides [IC-111]
Deven Paul Estes, *Christophe Copéret,* ETH Zurich

Catalytic Dehydrogenation of Amino Boranes – Formation of Condensed Borazine Compounds [IC-112]
Fabian Müller, *Hansjörg Grützmacher,* ETH Zurich

Cycloaddition Reactions of Diazoalkane Ruthenium Complexes with Chiral PNNP Ligands [IC-113]
Joël Egloff, *Antonio Mezzetti,* ETH Zurich

Synthesis and Application of N-Trifluoromethyl N-Heterocyclic Carbene Ligands and Their Complexes [IC-114]
Pascal Engl, *Antonio Togni,* ETH Zurich

Iron(II) Catalysts with a P-Stereogenic NPPN Ligand for the Enantioselective Strecker Reaction of Azomethine Imines [IC-115]
Raffael Huber, *Antonio Mezzetti,* ETH Zurich

Low temperature synthesis of nickel silicide: from preparing colloidal nanoparticles to coating silicon [IC-116]
Tsung-Han Lin, *Christophe Copéret,* ETH Zurich

Quantitatively Analyzing Metathesis Catalyst Activity and Structural Features in Silica-Supported Tungsten Imido–Alkylidene Complexes [IC-117]
Victor Mougel, *Christophe Copéret,* ETH Zurich

Amorphous Cobalt Silicate Nanobelts@Carbon Composites as Stable Anode Material for Lithium Ion Batteries [IC-118]
Wei Cheng, ETH Zurich

High Resolution Powder X-ray Diffraction on Functional Metal-Organic Frameworks with UiO-66 Topology [IC-119]
Marco Taddei, PSI Villigen, *Jeroen Anton van Bokhoven, ETH Zurich*

Synthesizing Functionalized $[M(\eta^6\text{-arene})_2]^+$ ($Re,^{99(m)}Tc$) Complexes for Receptor Targeting [IC-120]
Giuseppe Meola, *Roger Alberto, University of Zurich*

Target Specific Multimodality Nanoparticles for (Nano) Medical Applications [IC-121]
Michel Wuillemin, *Henrik Braband, University of Zurich*

Structural and magnetic investigations of a mononuclear 4f polyoxometalate family with single molecule magnet behaviour [IC-122]
Robin Güttinger, *Pierre-Emmanuel Car, University of Zurich*

Exceptionally long-lived light-emitting electrochemical cells: multiple intra-cation π-stacking interactions in $[Ir(C\hat{}N)_2(N\hat{}N)][PF_6]$ emitters [1] [IC-123]
Andreas M. M. Bünzli, University of Basel

Porphyrin-decorated polypyridines for dye sensitized solar cells [IC-124]
Angelo Lanzilotto, *Edwin C. Constable,* University of Basel

Asymmetric copper(I)-based dyes to combine with sterically demanding anchoring ligands for dye-sensitized solar cells. [IC-125]
Annika Büttner, *Edwin C. Constable,* University of Basel

Going to Extremes: From Fluorine-Free Blue to Stable Red Emitting Iridium Complexes for LEECs [IC-126]
Cathrin D. Ertl, *Edwin C. Constable,* University of Basel

Anionic Ir(III) Complexes for Light-Emitting Electrochemical Cells [IC-127]
Collin D. Morris, *Catherine E. Housecroft,* University of Basel

Influence of a co-adsorbent on the performance of copper(I)-based dye-sensitized solar cells [IC-128]
Frederik J. Malzner, *Edwin C. Constable,* University of Basel

Rhodium-catalyzed Olefin Cyclopropanation by Engineered Streptavidin [IC-129]
Jingming Zhao, *Thomas R. Ward*, University of Basel

Strong, Chemically Robust Photoreductants [IC-130]
Laura A. Büldt, University of Basel, *Oliver S. Wenger, Basel*

Modifying spacers and anchoring groups for heteroleptic Cu(I) - 6,6'-dimethyl-2,2'-bipyridine based DSSCs [IC-131]
Maximilian Klein, *Edwin C. Constable,* University of Basel

Heteroleptic light-emitting copper(I) complexes for possible applications in LECs and OLEDs [IC-132]
Sarah Keller, *Catherine E. Housecroft,* University of Basel

The Performance of a Series of Copper(I) Phenanthroline Dyes in DSCs [IC-133]
Sebastian Olivier Fürer, *Catherine E. Housecroft,* University of Basel

Tuning the in vitro cell cytotoxicity of dinuclear arene ruthenium trithiolato complexes: Influence of the arene ligand [IC-134]
Lennart Geiser, University of Bern

Synthesis, reactivity and cytotoxicity of dithiolato diruthenium complexes [(η^6-*p*-cymene)$_2$Ru$_2$(μ_2-SR)$_2$X$_2$], X = Cl, I [IC-135]
Lennart Geiser, University of Bern

Did the presence of a guest in the cavity of an arene ruthenium metallaprism modify its reactivity towards biomolecules? [IC-136]
Lydia Paul, *Julien Furrer,* University of Bern

Synthesis of metal oxide precursors for the generation of oxides or similar nanomaterials for Na-ion battery cathode production [IC-137]
Benoît Baichette, *Katharina Fromm, University of Fribourg*

Stimuli responsive cavitands for triggered release of antimicrobial drugs [IC-138]
Noémie Voutier, *Katharina Fromm,* University of Fribourg

Sn/C composite anode material for lithium ion batteries [IC-139]
Sivarajakumar Maharajan, *Katharina Fromm,* University of Fribourg

Pyridine versus pyrazine in asymmetric didentate ligands: unexpected behaviour in Fe^{II} spin crossover complexes [IC-140]
Timothée Lathion, *Claude Piguet,* University of Geneva

Synthesis of heteroaryl *meso* substituted porphyrins, and their coordination with ruthenium complexes [IC-141]
Balazs Brem, University of Neuchâtel, *Luminita Silaghi-Dumitrescu, Babes-Bolyai University*

Anti-Cancer Activities of Zwitterion-Bridged Arene Ruthenium Metalla-Assemblies [IC-142]
Minghui Yuan, *Bruno Therrien,* University of Neuchatel

Poly *versus* Mono-Disperse Rodlike Lipophilic Fluoroacetylacetonate Eu(III) Complexes: Mesomorphic and Thermodynamic Consequences [IC-143]
Sebastiano Guerra, University of Neuchatel, *Claude Piguet, University of Geneva*

Water-soluble organometallic assemblies containing photo-switchable ligands [IC-144]
Thomas Cheminel, *Bruno Therrien,* University of Neuchatel

Efficient Triplet Blue Emitters Based on Neutral Gold(III) Complexes [IC-145]
Alexander Szentkuti, *Koushik Venkatesan,* University of Zurich

Investigating the structure of the metallothionein 2 protein from the plant *Cicer arietinum* [IC-146]
Alma Salim, *Eva Freisinger,* University of Zurich

Highly Homoperfluorinated Ionic Liquids for NMR Field Probes for Magnetic Field Monitoring in MRI [IC-147]
Anna Christina Looser, *Roger Alberto,* University of Zurich

Photocatalytic Proton Reduction with Molecular Ru and Co Complexes Immobilized on Hydrophobic Silica [IC-148]
Cyril Bachmann, *Roger Alberto,* University of Zurich

Unique histidine-rich metallothioneins – "cracking the code" [IC-149]
Jelena Habjanic, *Eva Freisinger,* University of Zurich

Tackling the structure of the metal binding domains of a plant metallothionein 3 [IC-150]
Jovana Jakovleska, *Eva Freisinger,* University of Zurich

Characterization of Mg^{2+} binding sites in the CPEB3 ribozyme studied by NMR spectroscopy. [IC-151]
Kenneth Adea, *Roland K.O. Sigel,* University of Zurich

Polyoxometalate catalysts for artificial photosynthesis [IC-152]
Kim Dimuth von Allmen, *Greta R. Patzke,* University of Zurich

B_{12} derivatives with a modified corrin structure [IC-153]
Lucas Prieto, *Felix Zelder,* University of Zurich

Influence of hetero-biaryl-ligands on the photophysical properties of [Re^{I}NCS(CO)$_3$diimine]-type photosensitizers. [IC-154]
Mathias Lukas Mosberger, *Roger Alberto,* University of Zurich

Covalently labeling of the *btuB* riboswitch with fluorophores for the studies at the single molecule level [IC-155]
Meng Zhao, *Roland K.O. Sigel,* University of Zurich

N-Heterocyclic Carbenes - Stabilizing Ligands for Various Oxidation States of Rhenium and Technetium [IC-156]
Michael Benz, *Henrik Braband,* University of Zurich

Pyrphyrin and Phenphyrin Scaffold Revisited: Physico-Chemical Properties and Photocatalysis [IC-157]
Stephan Schnidrig, *Roger Alberto, University of Zurich*

A General Approach of Reduced Graphene Oxide Nanocomposite Aerogels with Multifunctional Electrode Materials towards Advanced Lithium-ion Batteries [IC-158]
Guobo Zeng, *Markus Niederberger*, ETH Zurich

Phosphine oxidation catalyzed by zerovalent cobalt complexes using nitrous oxide as oxidant [IC-159]
Thomas Lucien Gianetti, *Hansjörg Grützmacher*, ETH Zurich

Multitopic precursors for oxide materials' synthesis [IC-160]
Alba Finelli, *Katharina M. Fromm,* University of Fribourg

Stability and reactivity of dinuclear thiolato-bridged arene ruthenium complexes and their interactions with biological ligands [IC-161]
David Stibal, *Georg Süss-Fink,* University of Neuchatel

Using Oxidative Quenching of a Copper Photosensitizer for Light-Driven Hydrogen Production [IC-162]
Johannes Windisch, *Roger Alberto,* University of Zurich

Peptide Backbone Vitamin B_{12} Derivative: a Biomimetic Model [IC-163]
Marjorie Sonnay, *Felix Zelder,* University of Zurich

Medicinal Chemistry & Chemical Biology [MC] Poster Session

Jury members: Leonardo Scapozza, University of Geneva, Cornelia Zumbrunn, Actelion, Christian Heinis, EPF Lausanne, Georg Jaeschke, F. Hoffman-La Roche

Siglec-8 – A Novel Target For Asthma [MC-101]
Blijke Suzanne Kroezen, Basel, *Beat Ernst, University of Basel*

Chemically defined chromatin and protein engineering via EPL to study histone ubiquitination on the single molecule level [MC-102]
Andreas Linus Bachmann, EPF Lausanne

Engineering of a specific probe for the visualization and analysis of bivalent epigenetic marks in living cells [MC-103]
Aurore Delachat, *Beat Fierz,* EPF Lausanne

The Power of the 'SCS': Improving the Pharmacological Properties of Peptide Therapeutics [MC-104]
Christopher Kourra, *Nicolai Cramer,* EPF Lausanne

An *"in vivo"* temperature dependence study of the protoporphyrine IX delayed fluorescence lifetime while measuring the oxygen partial pressure. [MC-105]
Emmanuel Louis Arthur Gerelli, *Georges Wagnières,* EPF Lausanne

HP1α dynamic binding to different compaction states of chromatin [MC-106]
Louise Bryan, *Beat Fierz,* EPF Lausanne

Tackling Malaria by Inhibiting the SHMT Enzyme [MC-107]
Geoffrey Schwertz, *François Diederich,* ETH Zurich

Investigation of an engineered AaLS-13 capsid and Identification of the encapsulation pathway for GFP (+36) by high mass MALDI MS analysis [MC-108]
Katharina Root, *Renato Zenobi,* ETH Zurich

Fluorine Scan at the Active Sites of Rhodesain and Human Cathepsin L: Enhanced Binding Affinity by Stacking of Fluorinated Phenyl Rings on Flat Dipeptide Fragments [MC-109]
Maude Giroud, *Franois Diederich,* ETH Zurich

***O^6*-Alkylguanine Post-lesion DNA synthesis by Y-family DNA polymerase ζ characterized with synthetic nucleosides [MC-110]**
Michael Heinrich Räz, *Shana Sturla,* ETH Zurich

Structural Characterization of Oligoproline [MC-111]
Patrick Wilhelm, *Helma Wennemers,* ETH Zurich

Cell Penetrating Peptides Based on an Oligoproline Scaffold [MC-112]
Philipp Raschle, *Helma Wennemers,* ETH Zurich

Oligoprolines as Scaffolds for Tumor Targeting with Hybrid Bombesin Analogues [MC-113]
Stefanie Dobitz, *Helma Wennemers,* ETH Zurich

Impact of minor groove alkylation on transcription by RNA polymerase II [MC-114]
Stefano Malvezzi, *Shana Sturla*, ETH Zurich

Novel azobenzene-derived visible light photoswitches for biological applications [MC-115]
Zbigniew Pianowski, Karlsruher Institut für Technologie (KIT)

Bacterial Resistance to Silver: The Role of SilE Protein [MC-116]
Valentin Chabert, *Katharina Fromm, University of Fribourg*

The use of phosphorylated peptides to explore the folding properties of the protein tau required for AT8 antibody recognition [MC-117]
Yves Jacquot, Université Pierre et Marie Curie, Paris, *Guy Lippens, University of Lille 1*

Pollen induced asthma - could small molecules in pollen exacerbate the protein-mediated allergic response? [MC-118]
Alen Bozicevic, *Matthias Hamburger,* University of Basel

Search for alternatives to copper in organic farming: Fungicidal activity of a *Juncus effusus* medulla extract and its active constituent, dehydroeffusol, against downy mildew and apple scab [MC-119]
Justine Ramseyer, *Matthias Hamburger,* University of Basel

Natural and semisynthetic antitrypanosomal sesquiterpene lactones from *Anthemis nobilis* [MC-120]
Maria De Mieri, *Matthias Hamburger,* University of Basel

Antagonizing Bacterial Adhesion – Hit Identification by a Dynamic Combinatorial Chemistry Approach [MC-121]
Priska Frei, *Beat Ernst,* University of Basel

It's better to bend than to break [MC-122]
Said Rabbani, *Beat Ernst,* University of Basel

Development of small molecular tools for the cellular study of adenosine A_1 receptors [MC-123]
Jennifer Hemmings, *Martin Lochner,* University of Bern

Fluorescent probes for the cellular study of the 5-HT_3A receptor – synthesis and evaluation of near-infrared probes [MC-124]
Jonathan Simonin, *Martin Lochner,* University of Bern

Peptide dendrimer as SiRNA transfection reagent [MC-125]
Marc Heitz, *Tamis Darbre,* University of Bern

Excess Electron Transfer in DNA Containing a Pyrenyl Donor and Multiple Stable Phenanthrenyl Base-Surrogates [MC-126]
Pascal Röthlisberger, *Christian Leumann,* University of Bern

Antimicrobial Cyclic Peptides with L,D- architecture Targeting *Pseudomonas aeruginosa* [MC-127]
Runze He, *Jean-Louis Reymond,* University of Bern

Synthesis of a Geminal Difluorinated Tricyclic Nucleoside Analog [MC-128]
Sibylle Frei, *Christian Leumann,* University of Bern

Synthesis of photo-crosslinking probes and their application for the site-selective chemical modification of the 5-HT_3 receptor [MC-129]
Thomas Jack, *Martin Lochner,* University of Bern

Design of 3D Protein Fingerprint and its Application to Map the Protein Data Bank [MC-130]
Xian Jin, *Jean-Louis Reymond*, University of Bern

QPD-BA, A Precipating Dye For Monitoring Hydrogen Peroxide In Living Cells [MC-131]
Eric Lindberg, *Nicolas Winssinger,* University of Geneva

Protein Glycoconjugation by bioorthogonal click chemistry [MC-132]
Takuya Machida, *Nicolas Winssinger,* University of Geneva

Platinum-Porphyrin Conjugates as Highly Phototoxic Agents against Human Cancer Cells [MC-133]
Bernhard Spingler, University of Zurich

RNA internal loop: suitable binding site for metallo-intercalators? [MC-134]
Elena Alberti, *Daniela Donghi,* University of Zurich

Secrets of *in vitro* RNA folding and splicing revealed by fluorescent PNA labels [MC-135]
Ilija Vukadin, *Roland K.O. Sigel,* University of Zurich

RNA and Oxaliplatin: Investigation of Possible Platinum Binding Sites [MC-136]
Marianthi Zampakou, *Daniela Donghi,* University of Zurich

Studies on the mode of action of cationic β-hairpin antibiotics [MC-137]
Matthias Urfer, *John A. Robinson,* University of Zurich

Towards *in vivo* splicing of group II intron ai5γ [MC-138]
Maya Gulotti-Georgieva, *Roland K.O. Sigel,* University of Zurich

Characterization of group II introns *retrohoming* site at the single molecule level [MC-139]
Mokrane Khier, *Roland K.O. Sigel,* University of Zurich

Correlation between structure and antimicrobial activity of chitosan-alkyl thiomers – a biological study [MC-140]
Simona Conti, *Greta Ricarda Patzke,* University of Zurich

Peptide Shuttle System to Deliver PNAs to their Place of Action [MC-141]
Susann Zelger-Paulus, *Roland K.O. Sigel,* University of Zurich

Roles of the continuous internal water pathway in G-protein-coupled receptors activations [MC-142]
Shuguang Yuan, Actelion Pharmaceuticals Ltd., *Horst Vogel, EPF Lausanne*

Molecular Mechanism of Ruthenium and Gold Anticancer Agents in the Allosteric Regulation of the Nucleosome Core Particle (NCP) [MC-143]
Giulia Palermo, *Ursula Röthlisberger,* EPF Lausanne

Bicyclic peptide that selectively inhibits MMP-2 [MC-144]
Maola Khan, *Christian Heinis,* EPF Lausanne

Long-Lived States of Pairs of Fluorine-19 Nuclei: a new Tool for Ligand-Protein Screening [MC-145]
Roberto Buratto, *Geoffrey Bodenhausen,* EPF Lausanne

Comparison of ^{18}F-labeled alpha and gamma-conjugated folate derivatives for tumor imaging using positron emission tomography (PET) [MC-146]
Silvan David Boss, *Simon Mensah Ametamey,* ETH Zurich

Human Biomonitoring Bridging Gaps between Medicine and Environment [MC-147]
Basem Shomar, Qatar Environment and Energy Research Institute (QEERI)

Palladium-mediated *Suzuki-Miyaura* coupling: an efficient method for the formation of therapeutically relevant protein conjugates [MC-148]
Anaëlle Dumas, Université Paris-Sud

Enzyme catalyzed sulfur-carbon bond formation by ergothioneine biosynthetic sulfoxide synthase [MC-149]
Kristina Goncharenko, *Florian Seebeck,* University of Basel

Electrostatic Effect Of Halogenation On The Thermodynamic Stability Of Rapid Insulin Analogs [MC-150]
Krystel El Hage, *Markus Meuwly,* University of Basel

Preventing aggregation of porphyrinic photosensitizers using a biodegradable triblock copolymer [MC-151]
Ilche Gjuroski, *Julien Furrer*, University of Bern

Why are Vesicles of the Artificial 1,3-Diamidophosholipid Pad-PC-Pad Mechanosensitive? [MC-152]
Dennis Müller, *Andreas Zumbühl,* University of Fribourg

Addressing the tempormandibular joint disorder [MC-153]
Etienne Stalder, *Andreas Zumbühl,* University of Fribourg

Computer-aided drug design unveils the structural requisites for selective GPBAR1 activation [MC-154]
Francesco Saverio Di Leva, University of Naples Federico II

NMR investigation of the human RNA BCL2 G-quadruplex: restricting folding dynamics [MC-155]
Alicia Dominguez-Martin, *Roland K. O. Sigel*, University of Zurich

Metal ion dependency and multimerization behavior of biologically relevant human RNA G-quadruplexes [MC-156]
Helena Guiset-Miserachs, *Roland K.O. Sigel,* University of Zurich

Structure - antimicrobial activity relationships of chitosan-alkyl thiomers [MC-157]
Matteo Croce, *Greta Ricarda Patzke,* University of Zurich

Real-time Characterisation of a Large, Catalytic and Dynamic RNA by Single Molecule Microscopy. [MC-158]
Mélodie C.A.S. Hadzic, *Roland K.O. Sigel,* University of Zurich

Pore size matters - A crowding study of ribozyme folding and activity [MC-159]
Richard Börner, *Roland K.O. Sigel,* University of Zurich

The binding mechanism between a B_{12}-specific RNA and its ligand coenzyme B_{12} [MC-160]
Sofia Gallo, *Roland K.O. Sigel,* University of Zurich

Organic Chemistry [OC]
Poster Session

Jury members: Martin Lochner, University of Bern, Amalia Poblador Bahamonde, University of Geneva, Jieping Zhu, EPF Lausanne, Jérôme Waser, EPF Lausanne

1-Alkynyltriazenes as Functional Analogues of Ynamides [OC-101]
Florian Gérald Perrin, *Kay Severin,* EPF Lausanne

Convergent Synthesis of Glycopeptide Dendrimer Biofilm Inhibitors based on the Chloroacetyl-Thioether-Cysteine (ClAc) Ligation [OC-102]
Gaëlle Michaud, *Jean-Louis Reymond,* University of Bern

Mechanism, Optimization and Scope studies of Rh(II) Catalyzed One-Step Multi-Component Macrocyclization Reactions [OC-103]
Daniele Poggiali, *Jérôme Lacour,* University of Geneva

Synthesis and application of tetrafluoroethylation reagents based on hypervalent iodine [OC-104]
Jiri Vaclavik, *Antonio Togni,* ETH Zurich

Synthesis of a Hydrogen-Bonded Quaterthiophene and its Use in Organic Field-Effect Transistors [OC-105]
Bilal Özen, *Holger Frauenrath,* EPF Lausanne

[4+2]-Annulations of Aminocyclobutanes [OC-106]
Daniele Perrotta, *Jérôme Waser,* EPF Lausanne

Synthesis of chiral Ruthenium-cyclopentadienyl complexes and application to formal [4+2] cyclizations of yne-enones [OC-107]
David Kossler, *Nicolai Cramer,* EPF Lausanne

Synthesis, Characterization and Application of Styrene-Functionalized Imidazolium Salts [OC-108]
Felix D. Bobbink, *Paul Dyson,* EPF Lausanne

Rhodium(III)-Catalyzed C-H Activation Rapid Access to Versatile Organic Molecules [OC-109]
Manh Van Pham, *Nicolai Cramer,* EPF Lausanne

Chiral Cyclopentadienyl-Iridium Complexes as Catalysts for Cycloisomerizations of *N*-tethered 1,6-Enynes [OC-110]
Michael Christian Dieckmann, *Nicolai Cramer,* EPF Lausanne

Annulation of strained Rings, a Usefull Tool for the Synthesis of Nucleoside Analogues [OC-111]
Sophie Racine, *Jérôme Waser,* EPF Lausanne

Vicinal Amino Alcohols Synthesis from Allyl Amines via in Situ Tether Formation and Pd-Catalyzed Carboetherification [OC-112]
Ugo Orcel, *Jérôme Waser,* EPF Lausanne

Total Synthesis of (±)-Aspidophylline A [OC-113]
Weiwu Ren, *Jieping Zhu*, EPF Lausanne

Synthesis and Properties of Quinone-Type Push–Pull Chromophores [OC-114]
Cagatay Dengiz, *François Diederich,* ETH Zurich

Stereoselective Organocatalytic Synthesis of Oxindoles with Adjacent Tetrasubstituted Stereocenters [OC-115]
Oliver Dieter Engl, *Helma Wennemers,* ETH Zurich

Synthesis of Tröger's Base Analogues via a Phase-Transfer-Catalyzed Double Aza-Michael Reaction Under Base-Free Conditions [OC-116]
Takuya Kamiyama, *Jan Cvengros,* ETH Zurich

Towards a Short Synthesis of (*R,R,R*)-α-Tocopherol [OC-117]
Thomas Netscher, F. Hoffmann-La Roche AG

Chiral verdazyl radicals for metal-organic functional assemblies [OC-118]
Mattia Poretti, *Olimpia Mamula-Steiner,* Haute Ecole d'Ingénierie et d'Architecture Fribourg

Hyaluronic Acid-Based Hydrogels for Drug Delivery [OC-119]
Roger Marti, School of Engineering and Architecture of Fribourg

Efficient Access to Functionalized Cyclobutanone Derivatives Using Cyclobuteniminium Salts as Highly Reactive Michael Acceptors and Dienophiles [OC-120]
Alexandre Lumbroso, *Alain De Mesmaeker,* Syngenta Crop Protection AG

Strigolactam: New potent strigolactone analogues for the germination of Orobanche Cumana [OC-121]
Alexandre Lumbroso, *Alain De Mesmaeker*, Syngenta Crop Protection AG

6π/10π-electrocyclization of ketene-iminium salts for the synthesis of substituted naphthylamines [OC-122]
Amandine Kolleth-Krieger, *Alain De Mesmaeker,* Syngenta Crop Protection AG

Asymmetric synthesis of (+)-GR-24 and the four stereoisomers of (+)-5-deoxystrigol using [2+2]-cycloadditions of ketene-iminiums to olefins [OC-123]
Pierre-Yves Dakas, *Alain De Mesmaeker,* Syngenta Crop Protection AG

Organocatalytic Atroposelective Aldol Condensation [OC-124]
Achim Link, *Christof Sparr,* University of Basel

Total Synthesis of Fidaxomicin [OC-125]
Elias Kaufmann, *Karl Gademann,* University of Basel

Preparation of Fidaxomicin Analogs via Total Synthesis [OC-126]
Hiromu Hattori, *Karl Gademann,* University of Basel

Setting the Hook for Specific Single Walled Carbon Nanotubes [OC-127]
Ina Bodoky, *Marcel Mayor,* University of Basel

Direct preparation of pyrrolizidines using imines and isonitriles [OC-128]
Isabel Patrizia Kerschgens, *Karl Gademann*, University of Basel

Chemical modification of peptide and proteins for UV postionization and quantum interference experiments [OC-129]
Jonas Schaetti, *Valentin Köhler,* University of Basel

Towards a Perylene-Based Cyclophane with Charge-Transfer Capability [OC-130]
Kevin Weiland, *Marcel Mayor,* University of Basel

Synthesis of a Diacetylene-Bridged Geländer-Type Oligomer [OC-131]
Linda Maria Bannwart, *Marcel Mayor,* University of Basel

Synthesis of an Unknown Tetracyclic Derivative of Norbornane [OC-132]
Lorenzo Delarue Bizzini, *Marcel Mayor,* University of Basel

Molecules in Gasphase: Synthesis of Multi-Porphyrin-Systems for Quantum Interference Experiments [OC-133]
Lukas Felix, *Marcel Mayor,* University of Basel

Rotational restricted and functionalized CBP derivatives for blue emitting OLEDs [OC-134]
Manuel Hellstern, *Marcel Mayor,* University of Basel

Total synthesis of Aeruginosin 828A [OC-135]
Manuel Scherer, *Karl Gademann,* University of Basel

Radical Cyclizations involving Aryl Azides as Radical Traps [OC-136]
Benjamin Wyler, *Philippe Renaud,* University of Bern

Lipid Linked Oligosaccharide (LLO) Analogues as Bacterial Oligosaccharyltransferase (OST) PgLB Substrates [OC-137]
Jérémy Boilevin, *Jean-Louis Reymond,* University of Bern

Synthesis of Nitrogen-Containing Macrocycles via α-Imino Diazo Intermediates [OC-138]
Alejandro Guarnieri Ibáñez, *Jérôme Lacour,* University of Geneva

Enantiospecific C-H Azidation and ensuing functionalization of Tröger Bases [OC-139]
Alessandro Bosmani, *Jérôme Lacour,* University of Geneva

A Series of Novel Redox Gradient Fullerenes in Triple-Channel Photosystems [OC-140]
Altan Bolag, *Stefan Matile,* University of Geneva

The Anion-π Interaction: A Tuneable Non-Covalent Interaction for Catalysis [OC-141]
Franois Nicolas Miros, *Stefan Matile,* University of Geneva

Twisted Push-Pull Fluorophores as Mechanosensitive Probes [OC-142]
Saeideh Soleimanpour, *Stefan Matile,* University of Geneva

Arylamine Tribenzopentaphenes: Versatile Synthesis and study of their Hole Mobility [OC-143]
Andrew H. Rice, University of Washington, Seattle, USA

Route to the controlled formation of prostaglandin double bonds [OC-144]
Katalin Molnár, BME Szerves Kemia es Technologia Tanszek

Towards a Total Synthesis of Fijiolide A [OC-145]
Christoph Heinz, *Nicolai Cramer,* EPF Lausanne

Molecular and Polymeric Nanostructures Based on a Novel AAA-DDD Triple Hydrogen Bonding Motif [OC-146]
Marcus Papmeyer, *Kay Severin,* EPF Lausanne

Revisiting the Suzuki Coupling Based on Volcano Plots and Linear Scaling Relations [OC-147]
Michael Busch, *Clemence Corminboeuf,* EPF Lausanne

Suzuki-Miyaura Cross-Coupling Reactions of Unactivated Alkyl Halides Catalyzed by a Nickel Pincer Complex [OC-148]
Thomas Di Franco, *Xile Hu,* EPF Lausanne

Towards the Total Synthesis of the 3-Acyltetramic Acid Antibiotics Bu-2313A/B [OC-149]
Claudio Bomio, *Karl-Heinz Altmann,* ETH Zurich

KAT ligation for 3D control in hydrogels using 2-photon microscopy [OC-150]
Dmitry Mazunin, *Marcy Zenobi-Wong,* ETH Zurich

Towards the Total Synthesis of Acalycixeniolide F [OC-151]
Leo Betschart, *Karl-Heinz Altmann,* ETH Zurich

Functional Cumulene-Based Molecular Materials [OC-152]
Przemyslaw Gawel, *François Diederich,* ETH Zurich

Synthesis, Characterization and Application of an Ethano-Tröger's Base Derived Electrophilic Fluorinating Reagent [OC-153]
Raul Pereira, ETH Zurich, *Veronique Gouverneur, University of Oxford*

Cyanomethylation of aryl halides by domino Suzuki/fragmentation reaction [OC-154]
Juraj Velcicky, Novartis Pharma AG

Stabilization of Non-Kekulé Triangulene [OC-156]
Michal Juricek, University of Basel

Multi-Catalyst Screening for the Asymmetric Morita-Baylis-Hillman Reaction by Mass Spectrometric Monitoring of the Back Reaction [OC-157]
Patrick Isenegger, *Andreas Pfaltz,* University of Basel

Helically Chiral Biradicaloid Polycyclic Aromatic Hydrocarbon [OC-158]
Prince Ravat, University of Basel

Concentration Controlled Synthesis of Molecular Daisy Chains – Towards [c2]Daisy Chains as Functional Materials [OC-159]
Sylvie Drayss-Orth, *Marcel Mayor,* University of Basel

Modular Synthesis, Functionalization and resolution of Cationic [6]HELICENES [OC-160]
Geraldine Labrador, *Jérôme Lacour,* University of Geneva

Online swiss army knife for organic chemists [OC-161]
Luc Patiny, EPF Lausanne

Structure Refinement of a β-Heptapeptide Using RDCs Measured in a Stretched PVA Gel in Methanol [OC-162]
Carla Rigling, *Marc-Olivier Ebert,* ETH Zurich

Peptide-Catalyzed Stereoselective Conjugate Addition Reactions of Aldehydes to Maleimides [OC-163]
Claudio Grünenfelder, *Helma Wennemers,* ETH Zurich

Enantioselective Aldol Reactions with Fluoromalonyl Halfthioesters as Masked Fluoroacetates [OC-164]
Jakub Saadi, *Helma Wennemers,* ETH Zurich

Physical Chemistry [PC]
Poster Session

Jury members: Hans Jakob Wörner, ETH Zürich, Marcel Drabbels, EPF Lausanne, Samuel Leutwyler, University of Bern

A dive into the Cytochrome b_6f complex via ultrafast spectroscopy. [PC-101]
Adrien Chauvet, *Majed Chergui,* EPF Lausanne

Revealing conformers of protonated tryptophan by IR-IR-UV triple resonance spectroscopy of cold ions [PC-102]
Aleksandr Y. Pereverzev, EPF Lausanne

Bond-selective chemisorption of methane isotopologues on Pt(111) [PC-103]
Ana Gutiérrez-González, *Rainer Beck,* EPF Lausanne

Ultrafast Electro-modulated Differential Absorption Spectroscopy of Methylammonium Lead Iodide Perovskite Thin Films: Evidence for Carriers Trapping and Accumulation at the Surface [PC-104]
Arun Aby Paraecattil, *Jacques-E. Moser,* EPF Lausanne

Cold ion spectroscopy reveals the exact structure of protonated helical peptides in the gas-phase. [PC-105]
Chiara Masellis, *Thomas R Rizzo,* EPF Lausanne

Femtosecond transient absorption spectroscopy of $CsPbX_3$ perovskite nanoparticles [PC-106]
F. G. Santomauro, *Majed Chergui,* EPF Lausanne

Photoinduced charge transfer mechanism in Diketopyrrolopyrrole(DPP) dye-sensitiezed solar cell [PC-107]
Heewon Bahng, EPF Lausanne

Spectroscopic studies of kinetically trapped conformations in the gas phase: the case of triply protonated bradykinin [PC-108]
Liudmila Voronina, *Thomas R Rizzo,* EPF Lausanne

State-to-state scattering of $CH_4(\nu_3)$ from Ni(111) and LiF(100) surfaces. [PC-109]
Maarten van Reijzen, *Rainer Beck,* EPF Lausanne

Infrared spectroscopy of mobility-selected H^+-Gly-Pro-Gly-Gly (GPGG) [PC-110]
Michael Z Kamrath, *Thomas R Rizzo,* EPF Lausanne

Electronic energy transfer in model peptides [PC-111]
Valeriu Scutelnic, *Thomas R. Rizzo,* EPF Lausanne

Pushing the limits of cold ion spectroscopy: structural characterization of protonated ubiquitin in the gas phase [PC-112]
Vladimir Kopysov, *Oleg V Boyarkin,* EPF Lausanne

Photoassociation of cesium atoms upon Rydberg excitation in a dense ultracold gas [PC-113]
Heiner Saßmannshausen, *Frédéric Merkt,* ETH Zurich

Precision Spectroscopy in Cold Molecules: The First Rotational Intervals of He^+_2 by High-Resolution Spectroscopy and Rydberg-Series Extrapolation [PC-114]
Luca Semeria, *Frédéric Merkt,* ETH Zurich

Continuous trap loading of Rydberg-Stark decelerated metastable helium using overlaid electric and magnetic traps [PC-115]
Matija Zesko, *Frédéric Merkt,* ETH Zurich

MQDT-assisted high-resolution spectroscopy of the Rydberg states of H_2 - ionization energy of H_2 and rovibrational structure of H_2+ [PC-116]
Maximilian Beyer, *Frédéric Merkt,* ETH Zurich

High-Resolution VUV-Absorption Spectroscopy using Phase Modulation [PC-117]
U. Hollenstein, *Frédéric Merkt,* ETH Zürich

Mapping the electronic states of small transition metal clusters by nonlinear spectroscopy [PC-118]
Martin Beck, *Peter Pal Radi*, PSI Villigen

Dissociation dynamics of dissolved CH_3I studied with time-resolved resonant inelastic X-ray scattering [PC-119]
Rok Bohinc, PSI Villigen

Femtosecond Time-resolved Spectroscopy in the Extreme Ultraviolet Spectral Range [PC-120]
Jakob Grilj, Stanford University School of Medicine, *Majed Chergui, EPF Lausanne*

Quantum-Logic Spectroscopy for Single Trapped Molecular Ions [PC-121]
Gregor Hegi, *Stefan Willitsch*, University of Basel

Towards hybrid trapping of cold molecules and cold molecular ions [PC-122]
Dominik Haas, *Stefan Willitsch,* University of Basel

Cold Ion-Neutral Reactions in Next-Generation Ion-Atom Hybrid Traps [PC-123]
Pascal Eberle, *Stefan Willitsch,* University of Basel

Ionic Liquids based on crown ether as electrolytes for batteries [PC-124]
Hervé YAO, *Katharina M. Fromm,* University of Fribourg

Electrons and ionic liquids - a novel approach to study electron scattering from nonvolatile compounds [PC-125]
Khrystyna Regeta, *Michael Allan*, University of Fribourg

Ligand exchange reactions with Palladium, Platinum doped Au25(SR)18 clusters [PC-126]
Annelies Sels, *Thomas Bürgi,* University of Geneva

Tracking Solvent Controlled Photoinduced Electron Transfer Using Broadband Fluorescence Up-Conversion [PC-127]
Arnulf Rosspeintner, *Eric Vauthey* University of Geneva

Ligand exchange reaction of chiral $Pd_2Au_{36}(SR)_{24}$ cluster [PC-128]
Bei Zhang, *Thomas Bürgi,* University of Geneva

Chiral Recognition in Bimolecular Photoinduced Electron Transfer [PC-129]
Christoph Nançoz, *Eric Vauthey,* University of Geneva

Excited-state dynamics of radical ions [PC-130]
Joseph Samuel Beckwith, *Eric Vauthey,* University of Geneva

Separation of chemical shifts and J-couplings using homodecoupled-DIAG spectra [PC-131]
Marta Brucka, *Damien Jeannerat,* University of Geneva

Ultrafast Intersystem-crossing Dynamics and Breakdown of the Kasha-Vavilov's Rule of Naphthalenediimides [PC-132]
Oleksandr Yushchenko, *Eric Vauthey,* University of Geneva

Time Resolved infrared spectroscopy of Ruthenium(II) tris-bipyridyl complexes [PC-133]
Qinchao Sun, *Andreas Hauser,* University of Geneva

Structural investigation of the HS to LS relaxation dynamics on the porous coordination network [Fe(pz) $Pt(CN)_4$]·xH_2O [PC-134]
Teresa Delgado, *Andreas Hauser,* University of Geneva

Marangoni flow driven maze solving [PC-135]
Rita Toth, EMPA

Identification of Gas-Phase-Active Reactive Intermediates in Thermal Decomposition of Organophosphorus Compounds [PC-136]
Shuyu Liang, EMPA, *Hansjörg Grützmacher, ETH Zurich*

Exact versus approximate methods for nonadiabatic quantum molecular dynamics induced by the interaction with the electromagnetic field [PC-137]
Aurélien Patoz, *Jiri Vanicek,* EPF Lausanne

Hyperpolarized *para*-ethanol [PC-138]
Daniele Mammoli, *Geoffrey Bodenhausen,* EPF Lausanne

Excitonic Effects and Optical Spectra of Single Walled Carbon Nanotubes for Biosensor Applications in Life Sciences and Medicine [PC-139]
Dejan M Djokic, *Ardemis A. Boghossian*, EPF Lausanne

Studying Xe Migration in Truncated Hemoglobin with Molecular Dynamics Simulations [PC-140]
Polydefkis Diamantis, EPF Lausanne, *Markus Meuwly, University of Basel*

Tunneling in molecules probed by high-resolution photoelectron spectroscopy [PC-141]
Katrin Dulitz, *Frédéric Merkt,* ETH Zurich

Spectroscopy of Rydberg Helium in Electric and Magnetic Fields [PC-142]
Ondřej Tkáč, *Frédéric Merkt,* ETH Zurich

Kinetics of platinum oxidation [PC-143]
Urs Hartfelder, *Jeroen Anton van Bokhoven,* ETH Zurich

Single walled Carbon nanotubes-based composites for hybrid organic photovoltaic application [PC-144]
Brahim Aïssa, Qatar Environment and Energy Research Institute (QEERI)

Gas-phase Microsolvation of an Adenine Analogue [PC-145]
Luca Siffert, *Samuel Leutwyler,* University of Bern

Jet-Cooled UV-Spectra and Nonradiative Relaxation Dynamics of N1-Substituted Cytosines [PC-146]
Maria A. Trachsel, *Samuel Leutwyler,* University of Bern

Unusually long-lived transient negative ion of c-C_4F_8O formed by electron impact ionisation [PC-147]
Radmila Janeckova, University of Fribourg

Directional Energy Migration in Nanoparticles of Crystalline Transition Metal Complexes [PC-148]
Elia Previtera, University of Geneva

Nanoparticle – polyelectrolyte composites: Enhanced IR absorption and electron transfer upon visible light illumination [PC-149]
Harekrishna Ghosh, *Thomas Bürgi,* University of Geneva

Concentration dependent kinetic model of the energy transfer of Eu^{2+} in $SrAl_2O_4$ including thermal quenching processes [PC-150]
Jakob Bierwagen, *Hans Hagemann,* University of Geneva

Gold nanowire fabrication with lipid nanotubes [PC-151]
Kristina Jajcevic, *Kaori Sugihara,* University of Geneva

Raman optical Activity of chiral (6,5) Single Walled Carbon Nanotubes [PC-152]
Martin Magg, University of Geneva, *Bruce R. Weisman, Rice University*

Development of membrane mechanosensors with characterization in giant unilamellar vesicles. [PC-153]
Roberto Diego Ortuso, *Kaori Sugihara,* University of Geneva

Charge transfer processes in a molecular pentad [PC-154]
Margherita Orazietti, *Peter Hamm,* University of Zurich

Polymers, Colloids & Interfaces [PCI] Poster Session

Jury members: Stephen Schrettl, EPF Lausanne, Dorina Opris, EMPA, Samuel Jones, EPF Lausanne

Transport of calcium ions through thick biomimetic polymer membranes [PCI-101]
Mihai Lomora, *Cornelia Gabriela Palivan,* University of Basel

Amphiphilic Hexayne Derivatives as Precursors for Atomically Dense Carbon Nanolayers [PCI-102]
Bjoern Schulte, *Holger Frauenrath,* EPF Lausanne

Development of functionalized hybrid hydrogels [PCI-103]
Francois Noverraz, *Sandrine Gerber,* EPF Lausanne

Supramolecular organogels based on boronate esters and imidazolyl ligands [PCI-104]
Nicolas Luisier, *Kay Severin,* EPF Lausanne

PEGylation of sodium alginate for tuning the properties of hydrogel microspheres [PCI-105]
Solène Passemard, *Sandrine Gerber*, EPF Lausanne

Light-Induced Fragrance Release from Microcapsules Containing 2-Oxoacetates [PCI-106]
Andreas Herrmann, Firmenich SA

Effect of Reactive Extrusion on the Morphology of Polymer Nanocomposites [PCI-107]
Shirin Shokoohi, Research Institute of Petroleum Industry

An investigation into thermal analysis methods of detection and quantification of oxidative degradation of PVC-coated constructional steel [PCI-108]
Rachel Louise Alexander, Swansea University UK

Structural characteristics of amyloid-like fibers issued from a human estrogen receptor α-derived peptide [PCI-109]
Yves Jacquot, Université Pierre et Marie Curie, Paris

H-Bonded Supramolecular Polymers Selectively Dispersing and Subsequent Releasing Single-Walled Carbon Nanotubes [PCI-110]
Guojun Ke, *Marcel Mayor*, University of Basel

Synthetic biocompartments with selective membrane permeability towards protons and monovalent cations [PCI-111]
Mihai Lomora, *Cornelia Gabriela Palivan,* University of Basel

Development of triggered nanoreactor platforms [PCI-112]
Tomaz Einfalt, *Cornelia Gabriela Palivan,* University of Basel

Phenanthrene Nanotubes [PCI-113]
Caroline D. Bösch, *Robert Häner,* University of Bern

The formation of large assemblies through single, non-covalently attached pyrene phosphates [PCI-114]
Markus Probst, *Robert Häner,* University of Bern

Hierarchical self-assembly of the DNA-grafted supramolecular polymers [PCI-115]
Yuliia Vyborna, *Robert Häner,* University of Bern

$Pt^{(0)}$ containing metallosupramolecular polymers [PCI-116]
Luis Miguel Olaechea, *Christoph Weder,* University of Fribourg

Incorporation of dithiomaleimide as mechanophores into polymers chain [PCI-117]
Marc Karman, *Christoph Weder,* University of Fribourg

Side reactions in polycondensation of aromatic amino acids [PCI-118]
Michael Badoux, *Andreas Kilbinger,* University of Fribourg

Synthesis of polymer-silver nanocomposites for biomedical applications [PCI-119]
Milene Tan, *Katharina Fromm,* University of Fribourg

Design of Ag@SiO_2 nanorattles for antimicrobial implant coatings [PCI-120]
Sarah-Luise Abram, *Katharina Fromm,* University of Fribourg

DNA complexation effect on a cyanine probe studied at liquid/water interfaces by SSHG [PCI-121]
Giuseppe Leonardo Licari, *Eric Vauthey,* University of Geneva

Large-scale self-assembled gold nanoparticle arrays and plasmonic-enhanced fluorescence [PCI-122]
Mahshid Chekini, *Thomas Bürgi,* University of Geneva

Dispersion stability of layered double hydroxide particles in the presence of polyelectrolytes [PCI-123]
Marko Pavlovic, University of Geneva

Inverse Schulze-Hardy Rule [PCI-124]
Tianchi Cao, *Michal Borkovec*, University of Geneva

Improved fiber diameter determination of nanofibers through image analysis using a hierarchical scaling approach [PCI-125]
Fabian Deuber, *Christian Adlhart,* Zurich University of Applied Sciences, ZHAW

Tuning the size and aspect ratio of arrays of silica nanochannels [PCI-126]
Nicola Zucchetto, *Dominik Brühwiler,* Zurich University of Applied Sciences, ZHAW

Surface Activity of Nanoparticle Suspensions at Interfaces [PCI-127]
Yong Zen Tan, *Andrei Honciuc,* Zurich University of Applied Sciences, ZHAW

Ellipsoid-Shaped Superparamagnetic Nanoclusters through Emulsion Electrospinning [PCI-128]
Markus B. Bannwarth, EMPA

Long-lived charge carriers in organic Nanowires [PCI-129]
Regina Judith Hafner, *Holger Frauenrath,* EPF Lausanne

Porous nitrogen-doped carbon materials generated from fractal gels for CO_2 capture [PCI-130]
Anna Beltzung, *Massimo Morbidelli,* ETH Zurich

Synthesis and characterization of homologous (non-) interacting (hybrid) dendronized polymers with tunable bulk properties [PCI-131]
Leon F. Scherz, *A. Dieter Schlüter,* ETH Zurich

Nanocrystals of Cesium Lead Halide Perovskites ($CsPbX_3$, X=Cl, Br, and I) Showing Bright Emission with Wide Color Gamut [PCI-132]
Loredana Protesescu, *Maksym Kovalenko,* ETH Zurich

Controlled synthesis and functionalization of AuTTF micro- and nanowire sensors [PCI-133]
Mario Lenz, *Petra Dittrich,* ETH Zurich

Insight into how vesicles control the course of a laccase-catalysed oligomerization reaction [PCI-134]
Sandra Luginbühl, *Peter Walde,* ETH Zurich

Stability of radiation grafted polymer electrolyte membranes for water electrolysis cells [PCI-135]
Albert Albert, PSI Villigen

Chemical functionalization of nanocelluloses: a route to functional materials [PCI-136]
Philippe Tingaut, EMPA

Intact flying nanoparticles for gas-phase investigations [PCI-137]
Almudena Gallego, University of Basel, *Markus Arndt, University of Vienna*

Surfactant-Free Polarity Tuned Polymeric Nanoparticles Prepared by Ultrasonic Emulsion-Polymerization [PCI-138]
Dalin Wu, University of Basel, *Andrei Honciuc, Zurich University of Applied Sciences, ZHAW*

Janus Dumbbells: A flexible template for colloidal chemistry [PCI-139]
Florian Guignard, *Marco Lattuada*, University of Fribourg

Stimuli-responsive azo-containing polymeric materials [PCI-140]
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