

University of Zurich
Department of Chemistry
Winterthurerstrasse 190
CH-8057 Zürich



Thu, 11 September 2014, 9:30 - 18:45

Fall Meeting 2014

09.45	Welcome and conference opening
	, e
09.55	KGF-SCS Distinguished Industrial Investigator Award Lec-
	ture 2014, Dr. Hans Ulrich Blaser
	«Looking Back on 35 Years of Industrial Catalysis»
10.30	Sandmeyer Award Lecture 2014, Dr. Harald Walter,
	Syngenta Crop Protection Münchwilen AG
	«Sedaxane, isopyrazam and solatenol: Novel broad-
	spectrum fungicides inhibiting succinate dehydrogenase
	(SDH) – synthesis challenges and biological aspects»
11.15	Parallel Session I incl. award / invited lectures (8 Sessions
12.45	Lunch and Poster Session
	Commercial Exhibition
15.00	Parallel Session II (8 Sessions)
17.00	Paracelsus Award Lecture 2014, Prof. Richard R. Schrock,
	Massachusetts Institute of Technology
	«The Olefin Metathesis Reaction - Approaching Fifty Year
	of Age»
18.00	Best Oral Presentation Awards (sponsored by Metrohm)
18.15	Best Poster Presentation Awards (sponsored by DSM)

http://scg.ch/fallmeeting2014/





doi:10.2533/chimia.2014.532

WELCOME TO THE SCS FALL MEETING 2014



Philippe Renaud



Hans Peter Lüthi

On behalf of the Division of Chemical Research of the Swiss Chemical Society, we welcome you to the 2014 Fall Meeting. We also welcome the presenters of the nearly six-hundred scientific contributions (posters, contributed lectures, invited lectures). Given its popularity, the Fall Meeting represents a major event for chemical research in Switzerland, offering a unique opportunity for graduate students, post-doctoral fellows and senior scientists from academia and industry to share the results of their research.

Chimia 68 (2014) 532-559 © Schweizerische Chemische Gesellschaft

This year, the event is hosted jointly by the ETH Zurich Department of Chemistry and Applied Biosciences and the University of Zurich, Department of Chemistry at the Irchel Campus.

As in previous years, we will have a number of invited lectures presented by distinguished scientists. This year's Paracelsus Award Lecture will be given by Nobel Laureate Prof. Richard R. Schrock (Massachusetts Institute of Technology). The KGF-SCS Distinguished Industrial Investigator and the Sandmeyer Award Lectures, delivered by Drs. Hans Ulrich Blaser (St. Gallen, formerly Ciba-Geigy, Novartis and Solvias) and Harald Walter (Syngenta Crop Protection Münchwilen AG) are also part of the plenary program. Other invited and award lectures, including the Grammaticakis-Neumann Award Lecture, will be delivered in the Parallel Sessions.

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

We are grateful to our sponsors for their continued support. This support is also an expression of the interest of industry in our research activities, many of which are carried out by young scientists. This year, we particularly welcome the Qatar Foundation and the Qatar Environment and Energy Research Institute (QEERI), who will present their ambitious programs in the areas of renewable energy and water processing.

We invite you to browse through the program and hope that the 2014 Fall Meeting will capture your interest. The newly introduced 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 the University of Zürich Irchel Campus on September 11! Your participation and your contribution to the scientific discussion will help to make the event a success

Prof. Philippe Renaud Chairman of the Division of Chemical Research

for everybody involved.

PD Dr. Hans Peter Lüthi Chairman of the Organizing Committee

DEAR PARTICIPANTS OF THE FALL MEETING OF THE SWISS CHEMICAL SOCIETY



Michael O. Hengartner

It is a long-lasting and valuable tradition of the Swiss Chemical Society to invite young chemists to its annual Fall Meeting. Graduate students and postdoctoral fellows from all over Switzerland meet to discuss and present their latest research results.

I am very impressed by the fact that again almost 600 scientific contributions have been submitted for this year's conference.

The 2014 Zurich Fall Meeting of the Swiss Chemical Society is organized by a joint team of scientists from the ETH Zurich and the University of Zurich, a great example of a productive collaboration for the benefit of science. I am proud that the Swiss Chemical Society decided to hold its meeting on our University's Irchel Campus. I am confident that you will find this to be an excellent venue for this conformation.

I welcome you to the University of Zurich and wish you an interesting and successful conference meeting with many high quality contributions, stimulating discussions, and a friendly atmosphere that will promote scientific collaboration as well as personal friendship.

Prof. Michael O. Hengartner President of the University of Zurich SCS FALL MEETING 2014, 68, Nr. 7/8 533

PROGRAM OVERVIEW

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

Time	Program		Lecture hall
09.00	Welcome coffee Registration and poster installation		Lichthof
09.45	Welcome and conference opening PD Dr. <i>Hans Peter Lüthi</i> , Chair SCS Fall Meeting Prof. Dr. <i>Bernhard Schmid</i> , Dean of the Faculty of Science, UZH		G 30
09.55	KGF-SCS Distinguished Industrial Investigator Award Lecture 2014 Dr. <i>Hans Ulrich Blaser</i> «Looking Back on 35 Years of Industrial Catalysis» [PS-002]		G 30
10.30	Sandmeyer Award Lecture 2014 Dr. <i>Harald Walter</i> , Syngenta Crop Protection Münchwilen AG «Sedaxane, isopyrazam and solatenol: Novel broad-spectrum fungicides inhibiting succinate dehydrogenase (SDH) - synthesis challenges and biological aspects» [PS-003]		G 30
11.15	Catalysis Science & Engineering [C] Computational Chemistry [C] Inorganic & Coordination Chemistry [II] Medicinal Chemistry & Chemical Biology Organic Chemistry [C] Physical Chemistry [P]	AS-001], [AS-014] [AS-016] CE-001], [CE-002], [CE-015], [CE-016] CC-001], [CC-013] [CC-016] C-001], [IC-014] [IC-016] MC-001], [MC-011] [MC-015] DC-001], [OC-013] [OC-016] PC-001], [PC-013] [PC-016]	G 95 G 20 G 85 G 30 G 19 G 45 G 40 G 55
12.45	Catalysis Science & Engineering [C] Computational Chemistry [C] Inorganic & Coordination Chemistry [II] Medicinal Chemistry & Chemical Biology Organic Chemistry [C] Physical Chemistry [P]	AS-101] [AS-135] CE-101], [CE-168] CC-101] [CC-136] C-101] [IC-163] MC-101] [MC-192] OC-101] [OC-187] PC-101] [PC-163] PI-101] [PI-139]	Lichthof Galleries Lichthof
15.00	Catalysis Science & Engineering [C] Computational Chemistry [C] Inorganic & Coordination Chemistry [II] Medicinal Chemistry & Chemical Biology Organic Chemistry [C] Physical Chemistry [P]	AS-021] [AS-027] CE-003], [CE-023] [CE-027] CC-021] [CC-027] C-021] [IC-027] MC-002], [MC-004], [MC-021] [MC-025] CC-002], [OC-023] [OC-027] CC-021] [PC-027] C1-002], [P1-023] [PI-027]	G 95 G 20 G 85 G 30 G 19 G 45 G 40 G 55
16.45	Break and coffee/refreshments		Lichthof
17.00	Paracelsus Award Lecture 2014 Prof. <i>Richard R. Schrock</i> , Massachusetts Institute of Technology «The Olefin Metathesis Reaction - Approaching Fifty Years of Age» [PS-004]		G30
18.00	Best Oral Presentation Awards (sponsored by Metrohm	Best Oral Presentation Awards (sponsored by Metrohm)	
18.15	Best Poster Presentation Awards (sponsored by DSM)		G 30
18.30	End of the conference		

GENERAL INFORMATION

Date: September 11, 2014, 09.00–18.45

Location: University of Zurich

Irchel-Campus

Winterthurerstrasse 190 CH-8057 Zurich

Chairman

PD Dr. Hans Peter Lüthi Laboratory for Physical Chemistry ETH Zurich Wolfgang-Pauli-Strasse 10 CH-8093 Zurich Tel.: +41 44 632 21 05 luethi@phys.chem.ethz.ch

On-site Organization

Dr. Ferdinand Wild Chemistry Department University of Zurich Winterthurerstrasse 190 CH-8057 Zurich Tel.: +41 44 635 46 46 fwild@aci.unizh.ch

Conference Secretariat

Swiss Chemical Society David Spichiger and Sarah Schmitz Schwarztorstrasse 9 CH-3007 Bern Tel.: +41 31 310 40 90 info@scg.ch

Organizing Committee

Chairmen

- PD Dr. Hans Peter Lüthi, ETH Zurich (Chairman)
- Prof. Philippe Renaud, University of Bern (co-Chairman)
- Dr. Ferdinand Wild, University of Zurich (co-Chairman)

Analytical Sciences

PD Dr. Stefan Schürch, University of Bern

Catalysis Science and Engineering

Dr. Davide Ferri, PSI Villigen

Computational Chemistry

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

Inorganic Chemistry

- Prof. Thomas R. Ward, University of Basel
- Prof. Kay Severin, EPF Lausanne

Medicinal Chemistry and Chemical Biology

Dr. Yves Auberson, Novartis (Medicinal Chemistry)

Organic Chemistry

- Prof. Cristina Nevado, University of Zurich
- Prof. Andreas Pfaltz, University of Basel

Physical Chemistry

- Prof. Hans Jakob Wörner, ETH Zurich
- Prof. Stefan Willitsch, University of Basel

Polymers, Colloids and Interfaces

- Prof. Christian Hinderling, ZHAW

Admission

Presenters (Poster and/or Talk)

- SCS Members: free of charge (she/he, whose name is underlined in the abstract)
- Non-members: CHF 250.00 (+VAT)

Participants

- SCS Members: free of charge
- Non-members: CHF 50.00 (+VAT). Pre-registered participants will receive an invoice in advance to avoid waiting at the checkin desk. Pre-registration is possible until August 28, 2014.

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 August 28, 2014.

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

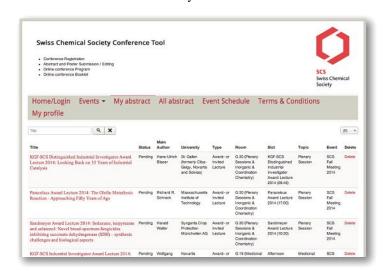
After the registration as a member, your login data can be used for the SCS Conference Tool as well.

Conference Tool



The new 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 details and profit from the following functions:

- Interactive program overview with abstract preview
- Quick abstracts display as html-file
- pdf-file download of abstracts directly to user's mailbox
- Extensive search functionality



Coffee Breaks and Lunch

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

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How to get to the Inchel Campus

The campus is easily accessible by public transportation (tram lines 7, 9, 10 and 14).

Go to www.sbb.ch and select *Zürich, Universität Irchel* or *Zürich, Milchbuck* as destination.

Departures from main station with InterCity, direction Zurich:

 Basel
 08:07

 Bern
 08:02

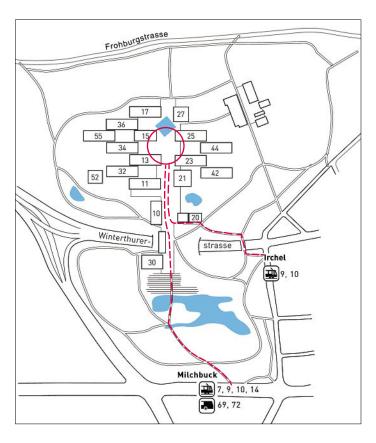
 Fribourg
 07:34

 Geneva
 06:14

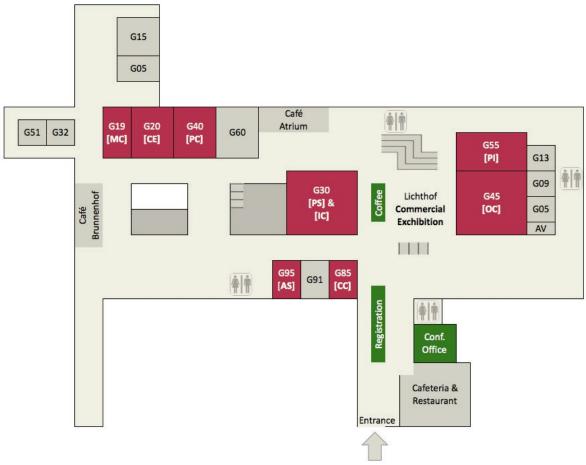
 Neuchatel
 07:27

 Lausanne
 06:47

 St.Gallen
 07:48



SITE MAP IRCHEL CAMPUS



The Fall Meeting 2014 is hosted and supported by:





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.







Member of Qatar Joundation งษอ จันแบ่งอ อ่างอ่อ





Best Oral Presentation Award

⚠ Metrohm

The prize is sponsored by Metrohm.

The prize is given for the two best presentations of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 18.00 in the 'Big Auditorium' (G30).

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.

Best Poster Presentation Award



The prize is sponsored by DSM.

The prizes were given for the best posters of each parallel session. The main criteria are the scientific quality and originality of the research, plus the quality of the presentation. Ceremony: 18.15 in the 'Big Auditorium' (G30).

Prizes for Winners

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

Prizes for Runners-up

- 1× runner-up prize for Analytical Sciences and Computational Chemistry Session,
- 2x runners-up prizes for Polymers, Colloids and Interfaces, Catalysis Sciences, Inorganic Chemistry and Physical Chemistry Session,
- 3× runners-up prizes for Medicinal Chemistry and Organic Chemistry Session
- Cash contribution of CHF 300.



Winners 2013, EPFL Lausanne



Winners 2013, EPFL Lausanne



The Qatar Environment and Energy Research Institute (QEERI)

is a member of Qatar Foundation for Education, Science and Community Development. QEERI plays a key role in addressing two of Qatar's national priorities: energy and water security. It seeks to address these grand challenges by undertaking long-term and multidisciplinary research and development in areas of solar energy, energy storage, smart grids, water desalination and reuse, and aquifer recharge. Join us on our exciting journey to help Qatar progress from a carbon-based to a knowledge-based economy.

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معهد قطر لبحوث البيئة والطاقة Qatar Environment & Energy Research Institute

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Session Endowments

Plenary Session

Givaudan^c

Givaudan Suisse SA

As the world's foremost fragrances and flavours business, Givaudan creates products that truly engage the senses, through innovating exquisite aromas and delicious tastes. Headquartered in Switzerland, Givaudan sources and develops ingredients for thousands of its customers' products and technologies, which are enjoyed every day by consumers around the world. Givaudan continually delivers new products and imaginative concepts, aided by a dedicated workforce of over 9,000 employees and operating in over 100 countries in all major markets, in both mature and developing regions.

[www.givaudan.com]

Computational Chemistry Session



IBM Research GmbH

IBM has maintained a research laboratory in Switzerland since 1956, located on its own campus in Rüschlikon near Zurich since 1962. As the European branch of IBM Research, the mission of the IBM Research Zurich lab – in addition to pursuing cutting-edge research for tomorrow's information technology – is to cultivate close relationships with academic and industrial partners, be one of the premier places to work for world-class researchers and to help drive Europe's innovation agenda. [http://www.zurich.ibm.com]

Catalysis Sciences & Engineering Session



Clariant International Ltd

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

[www.clariant.com]

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 'Lichthof' of the Irchel Campus, right after the registration and in front of the big auditorium and the coffee/lunch bench.



http://www.advion.com/



http://www.bruker.com/



http://www.agilent.ch/



https://www.brunschwig-ch.com/



http://www.borer.ch/

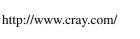


http://www.buchi.ch/



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http://www.gmp.ch/



http://www.lot-qd.de/ch/

🕰 Metrohm

http://metrohm.ch/



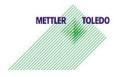
http://www.equilabo.com/



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http://www.mt.ch/



http://www.faust.ch/



http://igz.ch/



http://www.merckmillipore.ch/



http://ch.mlt.com/



http://www.perkinelmer.com/

For the Better



http://www.portmann-instruments.ch/



http://www.alfa.com



http://www.shimadzu.ch/



https://www.thieme.de/

Award Lectures Overview

09:55 Hans-Ulrich Blaser, St. Gallen (formerly Ciba-Geigy, Novartis and Solvias) is awarded the KGF-SCS Distinguished Industrial Investigator Award 2014 for his outstanding contributions to the development of highly selective and efficient catalysts for the industrial production of bioactive chiral compounds and for the leading role he played in asymmetric catalysis in both industry and academia.

«Looking Back on 35 Years of Industrial Catalysis» [PS-002]; Lecture hall G30

10:30 Harald Walter, Hans Tobler, Camilla Corsi and Denis V. Gribkov, Syngenta Crop Protection Münchwilen AG are awarded the Sandmeyer Award 2014 for their successful and innovative efforts in discovering, developing, and producing new broadspectrum agrochemical fungicides.

«Sedaxane, isopyrazam and solatenol: Novel broad-spectrum fungicides inhibiting succinate dehydrogenase (SDH) – synthesis challenges and biological aspects» [PS-003]; Lecture hall G30

11:15 Andreas Natsch, Givaudan Schweiz AG is awarded the KGF-SCS Industrial Investigator Award 2014 for his thorough investigation into the chemistry, biochemistry and microbiology of axilla malodor, culminating in the suppression of malodor causing processes and in the development of bacterial fragrance release from new families of odorant precursors.

«The human scent: Chemicals, enzymes and genes and our 'olfactive self'» [OC-001]; Lecture hall G45

11:15 *Erwin Reisner*, University of Cambridge, UK is awarded the Grammaticakis-Neumann Award 2014 for his research combing synthesis, photochemistry, photophysics, and molecular photobiology to develop artificial photosynthesis.

«Protein film photoelectrochemistry of the water oxidation enzyme Photosystem II» [CE-001]; Lecture hall G20

16:15 Werner Neidhart, F. Hoffmann-La Roche AG is awarded the KGF-SCS Senior Industrial Investigator Award 2014 for his contributions to medicinal chemistry and the creation of multiple candidate drugs, particularly Endothelin antagonists Avosentan and Clazosentan and the marketed Bosentan/Tracleer.

«Challenges & Rewards in Medicinal Chemistry Targeting Cardiovascular & Metabolic Diseases» [MC-003]; Lecture hall G19

16:35 Wolfgang Jahnke, Novartis Institutes for Biomedical Research is awarded the KGF-SCS Industrial Investigator Award 2014 for his excellence in developing and applying biomolecular NMR spectroscopy and fragment-based lead discovery, resulting in crucial contributions to many drug discovery projects.

«Contributions of biomolecular NMR to drug discovery» [MC-004]; Lecture hall G19

17:00 **Richard R. Schrock**, Massachusetts Institute of Technology is awarded the Paracelsus Award 2014 for his seminal work in synthetic and mechanistic organo-transition metal chemistry.

«The Olefin Metathesis Reaction - Approaching Fifty Years of Age» [PS-004]; Lecture hall G30

Plenary Sessions - G30



Chair: Prof. Dr. E. Peter Kündig

Session Endowment: Givaudan Suisse SA

09:55 KGF-SCS Distinguished Industrial Investigator Award Lecture 2014: Looking Back on 35 Years of Industrial Catalysis [PS-002]

Hans-Ulrich Blaser, St. Gallen (formerly Ciba-Geigy, Novartis and Solvias)

10:30 Sandmeyer Award Lecture 2014: Sedaxane, isopyrazam and solatenol: Novel broad-spectrum fungicides inhibiting succinate dehydrogenase (SDH) – synthesis challenges and biological aspects [PS-003]

Harald Walter, Syngenta Crop Protection Münchwilen AG

17:00 Paracelsus Award Lecture 2014: The Olefin Metathesis Reaction - Approaching Fifty Years of Age [PS-004]

Richard R. Schrock, Massachusetts Institute of Technology

Abstract codes

[XY-001][XY-009] [XY-011][XY-019]	Award or invited lecture Morning session lecture
[XY-021][XY-029]	Afternoon session lecture
[XY-031][XY-039]	Short poster presentations
[XY-101][XY-199]	Poster

AS Analytical Sciences
CC Computational Chemistry
CE Catalysis Sciences & Engineering
IC Inorganic Chemistry
MC Medicinal Chemistry & Chemical Biology
OC Organic Chemistry
PC Physical Chemistry

PI Polymers Colloids & Interfaces

PS Plenary Session

Name = Presenting Author Name = Research Leader

PARALLEL SESSIONS

Analytical Sciences [AS] Morning Session – G95

Chair: Dr. Stefan Schürch

Session Endowment:

11:15 Chemical Analysis by Mass Spectrometry in Space

– Initial Results from the Comet ChuryumovGerasimenko [AS-001]

Kathrin Altweg, University of Bern

12:00 Microscale probing and patterning of biological surfaces using nested hydrodynamic flow confinement and recirculation of sub-microliter volumes of liquid [AS-014]

Govind Kaigala, IBM Research GmbH

12:15 A Droplet Microfluidic ICP-MS Sample Introduction System [AS-015]

Pascal Emilio Verboket, Petra Dittrich, ETH Zurich

12:30 Electrostatic Spray Ionization Mass Spectrometry for Biochemical Analysis and Imaging [AS-016] Liang Qiao, *Hubert Girault*, EPFL Lausanne

Afternoon Session - G95

Chair: Dr. Marc Suter

Zurich

15:00 **2D-algal arrays on-chip as a tool for environmen- tal biosensing [AS-021]**

Coralie Suscillon, Vera Slaveykova, University of Geneva

15:15 Quantification of ghrelin and des-acyl ghrelin in human plasma by using cubic selected reaction monitoring LC-MS [AS-022]

Jonathan Sidibé, *Gérard Hopfgartner*, University of Geneva

15:30 Laser based N₂O isotopomer analysis bridges the gap between pure culture studies and field applications [AS-023]

Ellen Gute, EMPA Dübendorf

15:45 Direct voltammetric As(III) sensing in natural waters on a gel integrated renewable gold nanoparticle microelectrode [AS-024]

Romain Touilloux, Eric Bakker, University of Geneva

16:00 Native ESI-MS: Buffer Concentration Effect on Protein-Ligand Binding Affinities [AS-025]
Agni Faviola Mika Gavriilidou, *Renato Zenobi*, ETH

16:15 Instrumentino: An open-source modular Python framework for controlling Arduino based experimental instruments [AS-026]
Joel Koenka, *Peter Hauser*, University of Basel

16:30 Capillary zone electrophoresis as a capable tool in endotoxin and carbohydrate analysis [AS-027]
Blanka Bucsella, *Franka Kálmán*, University of Applied Sciences and Arts Northwestern Switzerland, FHNW

Computational Chemistry [CC] Morning Session – G85

Chair: Prof. Jürg Hutter



Session Endowment: IBM Research GmbH

11:15 Light Matter Interaction: The role of quantum coherence in energy transfer [CC-001]
Sabre Kais, Qatar Environment and Energy Research Institute, Doha, Qatar

11:45 Reviving geminal wavefunction theory: Accurate description of strong electron correlation at mean-field computational cost [CC-013]

Peter Limacher, Paul W. Ayers, McMaster University

12:00 Four-Component Density Matrix Renormalization Group [CC-014]
Stefan Knecht, Markus Reiher, ETH Zurich

12:15 Implementation of exact and approximate methods for nonadiabatic quantum molecular dynamics induced by the interaction with the electromagnetic field [CC-015]

Aurélien Patoz, Jiri Vanicek, EPFL Lausanne

12:30 **Towards Intramolecular SAPT [CC-016]**Antonio Prlj, Clemence Corminboeuf, EPFL Lausanne

Afternoon Session - G85

Chair: Prof. Markus Reiher

Geneva

15:00 Full-dimensional quantum dynamics and spectroscopy of ammonia isotopomers [CC-021]
Csaba Fábri, *Martin Quack*, ETH Zurich

15:15 Learning the error: Augmenting legacy quantum chemistry with machine learning [CC-022]
Raghunathan Ramakrishnan, University of Basel

15:30 Unravelling the stabilization mechanism of Aldoped Li-ion conducting Garnets by first-principle simulations. [CC-023]

Teodoro Laino, IBM Research GmbH

15:45 **Ab-initio Simulation of two-dimensional Networks on the Surface of Water [CC-024]** Ralph Koitz, *Jürg Hutter*, University of Zurich

16:00 Re-Engineering the B1 Domain of Streptococcal Protein G (GB1): Teaching an Old Dog New Tricks [CC-025]

Esra Bozkurt, Ursula Röthlisberger, EPFL Lausanne

16:15 Reactive Processes onto the Multidimensional Potential Energy Surface: Molecular Dynamics of the MbNO system [CC-026]
Maksym Soloviov, Markus Meuwly, University of

Basel

Anion-π_ and cation-_π interactions on the same aromatic surface [CC-027]

Marie Humbert-Droz, Stefan Matile, University of

Catalysis Sciences & Engineering [CE] Morning Session – G20 Chair: Dr. Davide Ferri

CLARIANT

Session Endowment: Clariant International Ltd

11:15 Grammaticakis-Neumann Award Lecture 2014:
Protein film photoelectrochemistry of the water
oxidation enzyme Photosystem II [CE-001]
Erwin Reisner, University of Cambridge, UK

11:45 Interplay between complexity and universality in industrial catalysts [CE-002]

Pascal Raybaud, IFP Energies nouvelles

12:15 C-H Activation on Tri-Coordinated Cr(III) Silica Surface Sites Initiates Ethylene Polymerization [CE-015]

Murielle F. Delley, Christophe Copéret, ETH Zurich

12:30 Transient studies of methane steam reforming over ceria-promoted Rh/Al₂O₃ [CE-016]

Afternoon Session - G20

Chair: Dr. Jeremy Luterbacher

15:00 Investigation of factors affecting the crystallisation of zeotype Sn-Beta with elemental mapping [CE-003]
Esben Taarning, Haldor Topsøe A/S

15:30 Mesopore quality determines the lifetime of hierarchically-structured zeolite catalysts [CE-023] Maria Milina, *Javier Pérez-Ramírez*, ETH Zurich

15:45 **1D and 2D Tuning of Cobalt-based Water Oxidation Catalysts [CE-024]**Fabio Evangelisti, *Greta Ricarda Patzke*, University of Zurich

16:00 Structured Fe₂O₃-based Catalyst for Reduction of Nitroarenes under Mild Conditions [CE-025] Oliver Beswick, *Lioubov Kiwi-Minsker*, EPFL Lausanne

16:15 NH₃ promoted formic acid decomposition over monolithic Au/TiO₂ catalyst: Rate enhancement without NH₃ oxidation [CE-026]

Manasa Sridhar, *Oliver Kröcher*, Paul Scherrer Institute, Villigen and EPFL Lausanne

16:30 Lactic acid production from biomass: a new chemocatalytic process compared to fermentation by LCA analysis [CE-027]
Pierre Dapsens, Javier Pérez-Ramírez, ETH Zurich

Inorganic & Coordination Chemistry [IC] Morning Session – G30 Chair: Prof. Thomas Ward



Session Endowment: Contact Group for Research Matters (KGF)

11:15 Nitrogenase: Mechanism and Applications
[IC-001]
Markus W. Ribbe, University of California, Irvine
(US)

12:00 Functionalised Clathrochelate Complexes –
New Building Blocks for New Supramolecular
Structures [IC-014]
Matthew Wise, Kay Severin, EPFL Lausanne

12:15 Iron Catalysts for Hydrogenation of Aldehydes: an Alternative to Precious Noble Metals [IC-015] Simona Mazza, *Xile Hu*, EPFL Lausanne

12:30 Synthesis, Structure and Reactivity of a Ruthenium Complex with an Unusual P₄Cl₂ Ligand [IC-016]

Mark Bispinghoff, Hansjörg Grützmacher, ETH Zurich

Afternoon Session - G30

Chair: Prof. Kay Severin

15:00 Supported alkene metathesis catalysts: from reaction intermediates to structure activity relationship [IC-021]

Victor Mougel, Christophe Copéret, ETH Zurich

15:15 Performance and in situ characterization of ceriabased non-stoichiometric oxides for the conversion of solar energy using two-step thermochemical cycles [IC-022] Matthäus Rothensteiner, Paul Scherrer Institute,

Matthäus Rothensteiner, Paul Scherrer Institute, Villigen, *Jeroen A. van Bokhoven*, ETH Zurich and Paul Scherrer Institute, Villigen

15:30 The surprising lability of homoleptic and heteroleptic bis-(2,2':6',2''-terpyridine) chromium(III) complexes [IC-023]

Jonas Schönle, Catherine E. Housecroft, University of Basel

15:45 Peptide Conjugates of Dinuclear Arene Ruthenium Trithiolato Complexes [IC-024]

Federico Giannini, University of Bern, Georg Süss-Fink, University of Neuchatel

16:00 Antimicrobial metal-containing Schiff base complexes [IC-025]

Sonja Kracht, Katharina Fromm, University of Fribourg

16:15 Aspects of the vibrational optical activity (VOA) of tetranuclear Cobalt transition metal complexes [IC-026]

Patric Oulevey, Thomas Bürgi, University of Geneva

16:30 X-ray structures of an octameric RNA duplex in the presence of six different divalent and trivalent metal ions reveal a particular innersphere binding to O4 of uracil [IC-027]

Michalla E. Schoffer, Boland K.O. Sigel, University

Michelle F. Schaffer, Roland K.O. Sigel, University of Zurich

Medicinal Chemistry & Chemical Biology [MC] Morning Session - G19



Chair: Prof. Jean-Louis Reymond

Session Endowment: Actelion Ltd

11:15 Engineering of high affinity probes for the visualization and analysis of bivalent epigenetic marks in living cells [MC-011] Aurore Delachat, Beat Fierz, EPFL Lausanne

11:30 Sphingosine-1-Phosphate Lyase Inhibitors as an Alternative Therapeutic Strategy to S1P-Receptor **Agonists for the Treatment of Multiple Sclerosis** [MC-012]

Berndt Oberhauser, Novartis Pharma AG

11:45 Disulfide-based prodrugs for improving the oral bioavailability of poorly water soluble drugs [MC-013]

Tao Sun, Jean-Christophe Leroux, ETH Zurich

12:00 Selective Aldosterone Synthase Inhibitors (ASI) - Design of an Orally Active Proof of Concept Compound [MC-014] Johannes Aebi, Kurt Amrein, F. Hoffmann-La Roche AG

Ru(II) Complexes and Photodynamic Therapy: 12:15 a Win-Win Combination [MC-015] Cristina Mari, Gilles Gasser, University of Zurich

12:30 Discovery of novel and highly selective allosteric inhibitors of PAK1 [MC-001] Alexei Karpov, Novartis Pharma AG

Afternoon Session - G19

Research

Chair: Dr. Heinz Fretz

15:00	Discovery of a potent P2Y ₁₂ receptor antagonist
	with an improved efficacy/safety profile [MC-021]
	Eva Caroff, Actelion Pharmaceuticals Ltd, Allschwil
15:15	Transannular cyclization of the sesquiterpene lac-
	tone nobilin into cadinanolide derivatives [MC-022]
	Maria De Mieri, <i>Matthias Hamburger</i> , University
	of Basel
15:30	From Synthesis in Flow to Integrated Dose-
	Response Screening in Flow [MC-002]
	Rainer E. Martin, F. Hoffmann-La Roche AG
15:45	Designed Cell Penetrating Peptide Dendrimers
	Efficiently Internalize Cargo into Cells [MC-024]
	Emilyne Blattes, Jean-Louis Reymond, University
	of Berne
16:00	Synthesis and fungicidal activity of quinolin-
	6-yloxyacetamides, a novel class of tubulin
	polymerization inhibitors [MC-025]
	Laura Quaranta, Syngenta Crop Protection AG
16:15	KGF-SCS Senior Industrial Investigator Award
	Lecture 2014: «Challenges & Rewards in
	Medicinal Chemistry Targeting Cardiovascular &
	Metabolic Diseases» [MC-003]
	Werner Neidhart, F. Hoffmann-La Roche AG
16:35	KGF-SCS Industrial Investigator Award Lecture
10.55	2014: «Contributions of biomolecular NMR to
	drug discovery» [MC-004]
	ui ug uiscovci y» [IVIC=UU+]

Wolfgang Jahnke, Novartis Institutes for Biomedical

Organic Chemistry [OC]

Morning Session - G45 Chair: Prof. Andreas Pfaltz



Session Endowment: Syngenta Crop Protection AG

11:15 KGF-SCS Industrial Investigator Award 2014: The human scent: Chemicals, enzymes and genes and our 'olfactive self' [OC-001] Andreas Natsch, Givaudan Schweiz AG

Highly Enantioselective Rh(I)-Catalyzed 11:45 **Activation of Cyclobutanones Enantiotopic C-C** Bond. [OC-013] Laetitia Souillart, Nicolai Cramer, EPFL Lausanne

12:00 Pd-catalyzed selective arylations of aldehydes [OC-014]

Ivan Franzoni, Clément Mazet, University of Geneva

12:15 **New Synthetic Applications of Nitrous Oxide** [OC-015] Gregor Kiefer, Kay Severin, EPFL Lausanne

12:30 **Pyridine Dearomatization Through Double Ru-Metal Carbene Insertions [OC-016]** Florian Medina, Jérôme Lacour, University of Geneva

Afternoon Session - G45

Chair: Dr. Henning Jessen

16:15

15:00 Sterol C(14)-demethylase inhibitors as fungicides for use in crop protection [OC-002] Sebastian Wendeborn, Syngenta Crop Protection AG 15:30 Difunctionalization of Activated Alkenes via Radical Addition/Desulfonylation/1,4-Aryl Migration Cascade Reaction [OC-023] Wangqing Kong, Cristina Nevado, University of Zurich **Total Synthesis of Aspidosperma Family** 15:45 **Monoterpene Indole Alkaloids [OC-024]** Olivier Wagnières, Jieping Zhu, EPFL Lausanne **Syntheses and Applications of Acylboronates** 16:00 in Chemoselective Amide Formations [OC-025] Hidetoshi Noda, Jeffrey W. Bode, ETH Zurich

Carbon Nanotubes (SWCNT) [OC-026] Ina Bodoky, Marcel Mayor, University of Basel 16:30 Rational Design of a Gold Carbene Precursor **Complex for a Catalytic Cyclopropanation**

Setting the Hook for Specific Single Walled

Reaction [OC-027] David Ringger, Peter Chen, ETH Zurich

Physical Chemistry [PC]

Morning Session – G40 Chair: Prof. Stefan Willitsch



Session Endowment: Bruker BioSpin

11:15	Bruker: Session Endowment Talk [PC-001]
	Guest speaker from Bruker Physik GmbH

- 11:45 **Attosecond photoelectron spectroscopy [PC-013]**Martin Huppert, *Hans Jakob Wörner*, ETH Zurich
- 12:00 Submm wave spectroscopy in the range 72 to 100 GHz of meta- and ortho-D-phenol: Probing tunneling switching dynamics
 [PC-014]
 Ziqiu Chen, Martin Quack, ETH Zurich
- 12:15 Control of chemical reactivity through spatial separation of molecular conformations [PC-015] Daniel Rösch, *Stefan Willitsch*, University of Basel
- 12:30 **Rydberg Spectroscopy of Zeeman-Decelerated Beams of Metastable Helium Molecules [PC-016]**Paul Jansen, *Frédéric Merkt*, ETH Zurich

Polymers, Colloids & Interfaces [PI] Morning Session – G55 Chair: Prof. Christian Hinderling



Session Endowment: Dow Europe GmbH

- 11:15 Observation of single-molecules at interfaces: fundamentals and applications [PI-001]

 Andrei Honciuc, Zurich University of Applied Sciences, ZHAW
- 11:45 **Stimuli-Responsive (Bio)Hybrid Coiled Coil Peptide–Polymer Microgels [PI-013]**Vitaliy Kolesov, *Harm-Anton Klok*, EPFL Lausanne
- 12:00 Organic-Inorganic Nanocomposite Scintillators:
 HfO₂: Eu Luminescent Nanoparticles Embedded
 into Polymer Films [PI-014]
 Alessandro Lauria, Walter Caseri, ETH Zurich
- 12:15 Modeling multiradicals in bulk crosslinking copolymerization [PI-015]
 Stefano Lazzari, ETH Zurich
- 12:30 Short Poster Presentations: Polymers, Colloids & Interfaces [PI-016]
 Chaired by Christian Hinderling, Zurich University of Applied Sciences, ZHAW

Afternoon Session - G40

Chair: Prof. Peter Hamm

- 15:00 Probing a Conformational Change of a
 Photoswitchable Allosteric Protein with Ultrafast
 IR Spectroscopy [PC-021]
 Brigitte Stucki-Buchli, Peter Hamm, University
 of Zurich
- 15:15 Light-induced charge transfer in the cytochrome bc₁ at high quantum yield [PC-022]
 Adrien Chauvet, *Majed Chergui*, EPFL Lausanne
- 15:30 Orientation and excited-state dynamics of DNA probes at liquid/water interfaces [PC-023]
 Giuseppe Leonardo Licari, *Eric Vauthey*, University of Geneva
- 15:45 Photoelectric conversion based on light induced proton pumps and proton-coupled electron transfer reactions [PC-024]
 Xiaojiang Xie, Eric Bakker, University of Geneva
- 16:00 Long-lived Charged Carriers in Oligothiophene Nanowires [PC-025]
 - Damien Rolland, Holger Frauenrath, EPFL Lausanne
- 16:15 Charge-transfer dissociation at organic donoracceptor interfaces probed with time-resolved electroabsorption [PC-026] Jelissa De Jonghe, *Jacques-E. Moser*, EPFL Lausanne
- Particle size and shape dependence of the ionic diffusivity in LiMnPO₄ cathode for lithium ion batteries [PC-027]

 Nam Hee Kwon, *Katharina Fromm*, University of Fribourg

Afternoon Session - G55

Chair: Prof. Dieter Schlüter

15:00 Generating anisotropic microstructures in colloidal gels [PI-002]

Jan Vermant, ETH Zurich

- 15:30 Tunable aggregation of sterically demanding peryleneimides induced by the conjugation with rigid oligoproline scaffolds [PI-023]
 Urszula Lewandowska, *Helma Wennemers*, ETH Zurich
- 15:45 Effect of hydrophobicity on nanoparticle formation: a case of ABC asymmetric triblock copolymers [PI-024]

 Evgenija Konishcheva Wolfgang Meier University

Evgeniia Konishcheva, Wolfgang Meier, University of Basel

16:00 Tandem Ring Opening-Ring Closing Metathesis for Synthesis of Functional Metathesis Catalysts [PI-025]

Amit Nagarkar, *Andreas Kilbinger*, University of Fribourg

16:15 The role of peptides in the formation of silver nanoparticles [PI-026]

Matthias Messerer, *Katharina Fromm*, University of Fribourg

16:30 Particle Aggregation in Ionic Liquids [PI-027]
Gregor Trefalt, *Michal Borkovec*, University of Geneva

POSTER SESSIONS

Name = Presenting Author
Name = Research Leader

Alphabetical ordered by presenting Author [XY-101]...[XY-199]

Analytical Sciences [AS] Poster Session

The Design of Selected Reaction Monitoring Method based on Empirical Spectra Library of Synthetic Peptides for Higher Sensitive Measurements [AS-101]

Bandar Alghanem, Gérard Hopfgartner, University of Geneva

HRMS dereplication, spectral networks and small molecule epigenetic modifiers: tools to decipher cryptic metabolic pathways in fungal microorganisms [AS-102]

Pierre-Marie Allard, Jean-Luc Wolfender, University of Geneva

Hyphenation of SPRi and MALDI MS for Interaction Analysis [AS-103]

Ulrike Anders, Renato Zenobi, ETH Zurich

MS-based isolation strategy for rapid targeted purification of antifungal compounds at the preparative scale [AS-104]

Antonio Azzollini, Jean-Luc Wolfender, University of Geneva

Evaluation of Hadamard Transform Atmospheric Pressure Ion Mobility-ESI-MS for the rapid profiling of isomeric natural products [AS-105]

Antonio Azzollini, Jean-Luc Wolfender, University of Geneva

Add-on Secondary Electrospray Ionizer for, delivering high ionization efficiency of vapors for the Analytical sector and for pre-existing API-M [AS-106]

Cesar Barrios-Collado, Pablo Martinez-Lozano Sinues, ETH Zurich

Exploring demultiplexing strategies for peptide identification in SWATH spectra: assessment of elution profile similarity [AS-107]

Aivett Bilbao, Gérard Hopfgartner, University of Geneva

Metabolite screening in plasma based on SWATH data acquisition in UHPLC-MS/MS analysis combined with a high resolution metabolomics library [AS-108]

Tobias Bruderer, *Gérard Hopfgartner*, University of Geneva

Analyzing Durable Anti-fungal Resistance Processes in Cereals by Metabolomics Using UHPLC-HR-MS [AS-109]

Rahel Bucher, Laurent Bigler, University of Zurich

Proton homodecoupling with enhanced resolution and sensitivity [AS-110]

Axelle Cotte, University of Geneva

Confined Thin Layer Cyclic Voltammetry for Halide Detection [AS-111]

Maria Cuartero, Eric Bakker, University of Geneva

Quantitation of Dystrophin in Quadriceps of Treated mdx Mice by LC-SRM/MS [AS-112]

Chantal Geiser, Stefan Schürch, University of Bern

Rapid and sensitive analysis of proteins with CE-SDS-LIF: mass spectrometric characterization of fluorescent labeled proteins [AS-113]

Miriam Goyder, HES-SO Valais, *Franka Kálmán*, University of Applied Sciences and Arts Northwestern Switzerland, FHNW

Quantification of La in CaMnO₃ by ICPMS for Analysis of PLD Films [AS-114]

Kevin Guex, Detlef Günther, ETH Zurich

Tandem mass spectrometric elucidation of the higher-order structure of sugar-modified nucleic acid duplexes [AS-115]

Yvonne Hari, Stefan Schürch, University of Bern

Method development for analysis of (oxygenised) volatile organic compounds in ambient air [AS-116]

Corinne C. Hoerger, Stefan Reimann, EMPA Dübendorf

Unraveling the requirements for immortality – Description of the alternative lengthening of telomeres type I cell phenotype using microarrays for mass spectrometry [AS-117]

Alfredo Ibanez, ETH Zurich

Investigation of Primaquine Metabolism and its Effects on the Metabolomic Distribution of Hepatocytes Using a Dedicated LC/MS Platform Including Automated Bligh & Dyer Extraction [AS-118]

Sandra Jahn, Gérard Hopfgartner, University of Geneva

Pattern-Based Sensing of Aminoglycosides [AS-119] Ziya Kostereli, EPFL Lausanne

Probing localized chemical phases in thin film solar cells [AS-120]

Wan-Ing Lin, Renato Zenobi, ETH Zurich

Scanning Carbonate Samples for Radiocarbon Content with Laser Ablation Coupled to Accelerator Mass Spectrometry [AS-121]

Caroline Münsterer, Detlef Günther, ETH Zurich

RASPPberry, an automated sample preparation platform [AS-122]

Inken Plitzko, F. Hoffmann-La Roche AG

Quantification of bufadienolides in Bryophyllum pinnatum leaves and manufactured products by UHPLC-ESI-MS/ MS [AS-123]

Olivier Potterat, Matthias Hamburger, University of Basel

At-line quantitative monitoring of the production of recombinant his-tagged proteins using fluorescence polarization [AS-124]

Denis Prim, *Jean-Manuel Segura*, University of Applied Sciences Western Switzerland Valais

Optimized strategy for an efficient Normal Phase MS-targeted isolation of natural products [AS-125] Davide Righi, *Jean-Luc Wolfender*, University of Geneva

Excess Electron Transfer Through Phenanthrenyl Base Pairs Within DNA [AS-126]

Pascal Röthlisberger, Christian Leumann, University of Bern

Nucleoside phosphate monitoring in mammalian cell fedbatch cultivation using quantitative matrix-assisted laser desorption/ionization time-of-flight mass spectrometry [AS-127]

Robert Steinhoff, Renato Zenobi, ETH Zurich

Zoom feature for a chemical microscope based on tip-enhanced Raman spectroscopy [AS-128] Jacek Szczerbiński, Renato Zenobi, ETH Zurich

1H HR-MAS NMR based metabolic profiling of cells in response to treatment with a hexacationic Ruthenium complex [AS-129]

Martina Vermathen, University of Bern

Fluorescent Sol based Optical Ammonia Gas Sensor [AS-130]

Susanne Widmer, EMPA St. Gallen, Lukas J. Scherer, Radiometer Basel

All Solid State Membrane Electrodes Based on Ferrocene Functionalized PVC [AS-131]

Zdenka Jarolímová, Eric Bakker, University of Geneva

Influence of the target plate material and sample layer thickness on LDI ionization efficiency for C60 [AS-132] Guido Paul Zeegers, Renato Zenobi, ETH Zurich

Ion-selective nanospheres as novel reagents in complexometric titrations [AS-133]

Jingying Zhai, Eric Bakker, University of Geneva

Application of SWATH acquisition method to the mass spectrometry-based proteomics study of monocyte-derived dendritic cells [AS-134]

Ying Zhang, Gérard Hopfgartner, University of Geneva

Instrumentino: An open-source modular Python framework for controlling Arduino based experimental instruments

Joel Koenka, Peter Hauser, University of Basel

Computational Chemistry [CC] Poster Session

Theoretical conformation analysis of a triazine-based, double decker rotor molecule with three anthracene blades

Maike Bergeler, Markus Reiher, ETH Zurich

A Density-Dependent Dispersion Correction: Beyond the post-SCF and ground state density [CC-102]

Eric Brémond, Clemence Corminboeuf, EPFL Lausanne

Computational study of the reaction between O(3P) and NO(2II) at temperatures relevant to the Hypersonic Flight Regime [CC-103]

Juan Carlos Castro-Palacio, Markus Meuwly, University of Basel

Understanding Supported Metallic Nanoparticles: An Ab Initio Approach [CC-104]

Aleix Comas-Vives, Christophe Copéret, ETH Zurich

Theoretical modeling of mesoporosity development in zeolites in alkaline media: Hierarchical ZSM-5 and ZSM-22 [CC-105]

Izabela Czekaj, Javier Pérez-Ramírez, ETH Zurich

Inter-system crossing with TDDFT: Jablonski diagrams from theory [CC-106]

Felipe Miraglia Franco de Carvalho, Ivano Tavernelli, EPFL Lausanne

Molecular scalar fields: From bonding descriptors to density functionals [CC-107]

Piotr de Silva, Clemence Corminboeuf, EPFL Lausanne

Monte Carlo Simulations of Bulk Liquid Water at Ambient Temperature and Pressure: Climbing the Jacob's Ladder of Density Functional Approximations [CC-108] Mauro Del Ben, University of Zurich

Liquid-liquid equilibrium and thermodynamics modeling of systems containing jatropha oil + methanol + glycerol + biodiesel [CC-109]

Kusumaningtyas Ratna Dewi, Semarang State University

Local density fitting within a Gaussian and plane waves approach [CC-110]

Dorothea Golze, University of Zurich

Ab Initio Modeling of TiO2-based Photo-catalysis for Water Reduction [CC-111]

Yeliz Guerdal, Jürg Hutter, University of Zurich

A new toolkit for fitting forcefield parameters used for Permanent Multipoles molecular simulations [CC-112] Florent Hédin, Markus Meuwly, University of Basel

LFDFT Calculations of Praseodymium doped binary Fluorides compared with Experimental Results [CC-113] Benjamin Herden, Claude A. Daul, University of Fribourg

Computational Investigations of Potential Water Oxidation Catalysts [CC-114]

Florian Hodel, Jürg Hutter, University of Zurich

Computation of Molecular Parity Violation in View of **Spectroscopic Experiments [CC-115]** Lubos Horny, Martin Quack, ETH Zurich

Interactive Visualization of PDB and CSD in 3D-Shape Space [CC-116]

Xian Jin, Jean-Louis Reymond, University of Bern

Excited state calculations with MPS-DMRG [CC-117] Sebastian Keller, Markus Reiher, ETH Zurich

Free-radical copolymerization of acrylamides, acrylates and α-olefins [CC-118]

Rollin King, Bethel University

Adaptive Tensor Network Parameterizations of the Electronic Wave Function for Application in Strong-**Correlation Problems [CC-119]**

Arseny Kovyrshin, Markus Reiher, ETH Zurich

Adjusting the Local Arrangement of π -Stacked Oligothiophenes to Promote Charge Transfer [CC-120] Hongguang Liu, Clemence Corminboeuf, EPFL Lausanne

Progress on DMRG-SCF Gradients for State-specific and **State-averaged Cases [CC-122]**

Yingjin Ma, Markus Reiher, ETH Zurich

Mechanism of ethylene polymerization by CrIII silicates via C-H activation: insights from DFT calculations [CC-123]

Francisco Nuñez Zarur, Christophe Copéret, ETH Zurich

Noncovalent interactions in isostrutural cocrystals and salts: A theoretical investigation [CC-124]

Nirmal Ram Jayaraman Selvaraj, *Tomasz Adam Wesolowski*, University of Geneva

Theoretical account of the electronic structure and properties of systems with two-open-shell f and d electrons [CC-125]

Harry Ramanantoanina, Claude A. Daul, University of Fribourg

The Subtle Effect of the Solvent on Competing Reaction Mechanisms Involving λ^3 -iodanes: From the Reaction Profile to the Minimal Energy Pathway on the Free Energy Surface [CC-126]

Oliver Sala, Antonio Togni, ETH Zurich

Chemoinformatics Meets Quantum Chemistry: A Strategy for Computational Molecular/Reaction Analysis Based on The Global Reaction Route Maps [CC-127] Hiroko Satoh, National Institute of Informatics, Tokyo

Non-uniform Continuum Model for Solvatochromism Based on Frozen-Density Embedding Theory [CC-128] Sapana Shedge, *Tomasz Adam Wesolowski*, University of Geneva

Excess electrons in anatase: a hybrid DFT and RPA study [CC-129]

Clelia Spreafico, ETH Zurich

Exciton coupling in π -stacked chromophores: a challenge for electronic structure approaches [CC-130]

Peter R. Tentscher, Clémence Corminboeuf, EPFL Lausanne

Dynamics of retinal chromophore in rhodopsin: from cis-trans isomerisation to activation [CC-131]

Siri Camee Van Keulen, *Ursula Röthlisberger*, EPFL Lausanne

Visualizing and quantifying interactions in the excited states using molecular scalar fields [CC-132]

Laurent Vannay, Clemence Corminboeuf, EPFL Lausanne

MD Simulations of Non-linear Hydrogen Transfer with Zero-point Energy Corrected MMPT Force Field [CC-133]

Zhen-Hao Xu, Markus Meuwly, University of Basel

Alchemical Coupling Approaches within Quantum Chemistry [CC-134]

K. Y. Samuel Chang, O. Anatole von Lilienfeld, University of Basel

On-the-fly ab initio semiclassical dynamics: Identifying degrees of freedom essential for emission spectra of oligothiophenes [1] [CC-135]

Marius Wehrle, EPFL Lausanne

Accelerating Quantum Instanton Calculations of Kinetic Isotope Effects [CC-136]

Konstantin Karandashev, EPFL Lausanne

Catalysis Sciences & Engineering [CE]
Poster Session

Efficient biphasic processing of sugars to furans over GaUSY/Amberlyst-36 in continuous mode [CE-101] Christof Aellig, *Javier Pérez-Ramírez*, ETH Zurich

Alkane Hydroxylation Using an Artificial Metalloenzyme Based on the Biotin-Streptavidin Technology [CE-102] Maxime Barnet, *Thomas R. Ward*, University of Basel

Pretreatment effect on supported Au_x(SR)_y clusters [CE-103] Noelia Barrabes, *Thomas Bürgi*, University of Geneva

Fe₂O₃-TiO₂ Nanostructured Composite Photoanode for Water Splitting [CE-104]

Mario Bärtsch, Markus Niederberger, ETH Zurich

Activated Carbon Fibers as Efficient Structured Adsorbent for VOCs Removal [CE-105]

Guillaume Baur, Lioubov Kiwi, EPFL Lausanne

Secondary reactions during the decomposition of formic acid [CE-106]

Amaia Beloqui Redondo, *Jeroen A. van Bokhoven*, ETH Zurich and Paul Scherrer Institute, Villigen

Towards Ocean Based Biorefinery: N-Acetyl-D-Glucosamine (NAG) to Value-Added Polyols. [CE-107]

Felix D. Bobbink, Paul Dyson, EPFL Lausanne

Controlling the active phase distribution in shaped catalysts [CE-108]

Lars Borchardt, Javier Pérez-Ramírez, ETH Zurich

Membrane reactor concept for CO₂ methanation [CE-109] Andreas Borgschulte, EMPA Dübendorf

Activation of Cu-mordenite for methane to methanol conversion: Effects of synthesis and multiple cycles on methanol production [CE-110]

Selmi Erim Bozbag, *Jeroen A. van Bokhoven*, ETH Zurich and Paul Scherrer Institute, Villigen

Protecting nano-particles against sintering for application under demanding catalytic conditions [CE-111]

Andrew Chang-Yin Chien, Paul Scherrer Institute, Villigen, Jeroen Anton van Bokhoven, ETH Zurich and Paul Scherrer Institute, Villigen

The Mechanism of (catalytic) Lignin Pyrolysis: Linking Model Compounds to Lignin [CE-112]

Victoria Custodis, Jeroen A. van Bokhoven, ETH Zurich

Esterification of Lignin Monomers and Fatty Acids using Separable Solid Acids [CE-113]

Bahir Duraki, Jeroen A. van Bokhoven, ETH Zurich

Increased methanation activity of ruthenium nanoparticles through passivation of the silica support [CE-114]

Karol Furman, Christophe Copéret, ETH Zurich

Identifying short-lived phases and their rates of formation and disappearance from transient XAS spectroscopy [CE-115]

Urs Hartfelder, Jeroen A. van Bokhoven, ETH Zurich

Studying the structure-directing effect of aromatic-functionalized templates in zeolite synthesis [CE-116]

Manuel Hernandez-Rodriguez, *Javier Pérez-Ramírez*, ETH Zurich

Controlled growth and interfaces of supported iridium nanoparticles via surface organometallic chemistry [CE-117]

Florent Héroguel, Christophe Copéret, ETH Zurich

Microwave-assisted nonaqueous synthesis of WO₃ nanoparticles for crystallographically oriented photoanodes for water splitting [1] [CE-118]

Sandra Hilaire, Markus Niederberger, ETH Zurich

Organometallic Chemistry with Metal-Organic Frameworks: Well-Defined Heterogeneous Catalytic Sites for Olefin Metathesis [CE-119]

Rifat Kamarudheen, Paul Scherrer Institute, Villigen, Jeroen A. van Bokhoven, ETH Zurich and Paul Scherrer Institute, Villigen

Structure modification and carbon resistance improvement of modified Ni/Al₂O₃ catalysts for synthetic natural gas production [CE-120]

Anastasios Kampolis, *Oliver Kröcher*, Paul Scherrer Institute, Villigen and EPFL Lausanne

Hydrogenation of Arenes by Metal Nanoparticles Combined with Lewis Acidic Ionic Liquids [CE-121]

Alena Karakulina, Paul Dyson, EPFL Lausanne

Single particle spectroscopy on well-defined models systems prepared using nanotechnology to study size-effects in catalysis [CE-122]

Waiz Karim, *Jeroen A. van Bokhoven*, ETH Zurich and Paul Scherrer Institute, Villigen

Post-synthetic design of basic zeolites for bio-oil upgrading [CE-123]

Tobias Keller, Javier Pérez-Ramírez, ETH Zurich

Oxidative coupling of methane on flame-made Mn-Na₂WO₄/ SiO₂: Influence of catalyst composition and reaction conditions [CE-124]

Rajesh Koirala, Alfons Baiker, ETH Zurich

Oxidative dehydrogenation of ethane (ODHE) with CO₂ over flame-made Ga-loaded TiO₂ [CE-125]

Rajesh Koirala, Alfons Baiker, ETH Zurich

In Situ Resonant X-Ray Emission Spectroscopy of Ce³⁺ Formation During CO Oxidation at Low Temperatures over Platinum Nanoparticles Supported on Ceria [CE-126]

René Kopelent, Olga V. Safonova, Paul Scherrer Institute, Villigen

Gas-phase selective oxidation of glycerol to dihydroxyacetone over iron zeolites [CE-127]

Giacomo Marco Lari, Javier Pérez-Ramírez, ETH Zurich

Electrocatalytic reduction of carbon dioxide by thiolprotected silver nanoclusters [CE-128]

Gastón Larrazábal, Javier Pérez-Ramírez, ETH Zurich

Rhodium doped ceria: Organics from sunlight, H_2O and CO, ? [CE-129]

Fangjian Lin, Paul Scherrer Institute, Villigen

Cobalt-based spinel catalysts for visible-light-driven water oxidation [CE-130]

Hongfei Liu, Greta Ricarda Patzke, University of Zurich

DRIFTS-HEROS study of CO oxidation on Pt catalysts [CE-132]

Valentina Marchionni, *Davide Ferri*, Paul Scherrer Institute, Villigen

Operando Monitoring of Surface Processes during Heterogeneous Asymmetric Hydrogenation of Ketones on Chirally-Modified Platinum Catalyst [CE-133] Fabian Meemken, Konrad Hungerbühler, ETH Zurich

Engineering Single-Sites Inside Metal Organic Frameworks in the Search for New Water Oxidation Catalysts [CF-134]

Kim Meyer, ETH Zurich, *Jeroen A. van Bokhoven*, ETH Zurich and Paul Scherrer Institute, Villigen

Scalable Enantioselective Synthesis of Fmoc- β^2 -Serin and -Threonin by Organocatalytic Mannich Reaction [CE-135]

Daniel Meyer, *Roger Marti*, School of Engineering and Architecture of Fribourg

WO₃-CeO_x-TiO₂ catalyst prepared by one-step flame spray synthesis for NO_x reduction in the NH₃-SCR [CE-136] Katarzyna Michalow-Mauke, *Oliver Kröcher*, Paul Scherrer Institute, Villigen and EPFL Lausanne

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- Sulfonamide Inhibitors of 2-Methylerythritol 2,4-Cyclodiphosphate Synthase (IspF) from Arabidopsis thaliana and Plasmodium falciparum [MC-181] Jonas Thelemann, François Diederich, ETH Zurich

- Factors influencing the uptake of biotinylated ruthenium complexes for in vivo catalysis in E.coli [MC-182] Christian Trindler, *Thomas R. Ward*, University of Basel
- New structure-activity relationship studies on bombesinbased tracers for tumor targeting [MC-183] Ibai Valverde, *Thomas L. Mindt*, University of Basel Hospital
- Investigation of the structure of LecA and multivalent ligands with crystallography and MD simulation [MC-184] Ricardo Visini, *Jean-Louis Reymond*, University of Bern
- Iron phosphate nanoparticles do not impair membrane integrity or metabolic activity in intestinal cell lines [MC-185]

Lea M von Moos, Shana Sturla, ETH Zurich

Metabolomic profiling of bovine cumulus cells and oocytes during in-vitro maturation of cumulus-oocyte complexes [MC-186]

Jasmin Walter, University of Zurich

3-Alkoxy-pyrrolo[1,2-b]pyrazolines as novel selective androgen receptor modulators (SARMs) with unique physicochemical properties for transdermal administration [MC-187]

Sven Weiler, Novartis Institutes for Biomedical Research

- Crystal Structure of an Oligoproline PPII-Helix [MC-188] Patrick Wilhelm, *Helma Wennemers*, ETH Zurich
- A synthetic nucleotide analog enables polymerase-mediated amplification of DNA containing promutagenic O°-alkylguanine adducts [MC-189]
 Laura Wyss, Shana Sturla, ETH Zurich
- A unifying framework for protein amyloid self-assembly: from protein-protein interactions to large-scale structures [MC-190]

Alessio Zaccone, University of Cambridge, Marco Lattuada, University of Fribourg

A new labelling strategy to visualize an RNA splicing process [MC-191]

Susann Zelger-Paulus, *Roland K.O. Sigel*, University of Zurich

Probing Capsid Dynamics with Protein FRET [MC-192]Reinhard Zschoche, *Donald Hilvert*, ETH Zurich

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Synthesis of Cyclopentenones by an Asymmetric Nickel-Catalyzed [3+2] Reductive Cycloaddition of Enoates with Alkynes [OC-101]

Joachim Ahlin, Nicolai Cramer, EPFL Lausanne

Mono-, Bis- and Penta-adducts of $M_3N@C_{80}$ (M = Y, Gd): Regioselective Addition Controlled by Endhedral Metal Clusters [OC-102]

Safwan Aroua, ETH Zurich

- Synthesis of functionalized pyridinium salts [OC-103] Johanna Auth, *Andreas Pfaltz*, University of Basel
- Synthesis of Porphyrins for Surface Chemistry and Materials Science [OC-104]

Jesse Bergkamp, Silvio Decurtins, University of Bern

Towards the total synthesis of Augustamine [OC-105] Lucile Bernet, *Christian Bochet*, University of Fribourg

Stabilization of Disfavored Conformations inside an Adaptive Self-Assembled ${\rm Fe_4L_4}$ Coordination Capsule ${\rm [OC-106]}$

Jeanne L. Bolliger, *Jonathan R. Nitschke*, University of Cambridge

- Cleavage of Aromatic C—O Bonds using Metal Nanoparticles in Aqueous Media [OC-107] Safak Bulut, *Paul Dyson*, EPFL Lausanne
- Enantioselective Michael Addition of Isocyanoactate to Vinyl Selenone: Access to α-Quaternary Amino Acids [OC-108] Thomas Buyck, *Jieping Zhu*, EPFL Lausanne
- Broadband Dye-Zeolite L Composites for Luminescent Solar Concentrators [OC-109]

Pengpeng Cao, Peter Belser, University of Fribourg

Artificial Suzukiase Based on the Biotin-Streptavidin Technology [OC-110]

Anamitra Chatterjee, Thomas R. Ward, University of Basel

Studies Towards the Total Synthesis of (2R)-Hydroxy-Norneomajucin [OC-111]

Erika Crane, Karl Gademann, University of Basel

- Metal Free Catalyst for Chemoselective Methylation of Amines Using CO₂ as a Methylating Agent [OC-112] Shoubhik Das, *Paul Dyson*, EPFL Lausanne
- **Towards Zwitterionic Charge-Transfer Janus Dendrimers** [OC-113]

Cagatay Dengiz, François Diederich, ETH Zurich

Towards a photochemically-promoted Native Chemical Ligation (PNCL) [OC-114]

Sebastian Dobarco, Christian Bochet, University of Fribourg

- Outstanding Chiroptical Properties: A Signature of Enantiomerically Pure Alleno-Acetylenic Macrocycles and Monodisperse Acyclic Oligomers [OC-115] Etienne Donckele, François Diederich, ETH Zurich
- Concentration controlled synthesis of Daisy Chains A [c2] daisy chain with the potential application as a molecular potentiometer [OC-116]

Sylvie Drayss, Marcel Mayor, University of Basel

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Samad Ebrahimi, Matthias Hamburger, University of Basel

Mono Thiomalonates in the Organocatalyzed Synthesis of 3,4-Dihydrocoumarins and 3,4-Dihydroquinolinones [OC-118]

Oliver Engl, Helma Wennemers, ETH Zurich

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Lukas Felix, Marcel Mayor, University of Basel

Electrophilic trifluoromethylation and the formation of quaternary stereogenic centers [OC-120]
Natalja Früh, *Antonio Togni*, ETH Zurich

Metal-Free Aryltrifluoromethylation of Activated Alkenes [OC-121]

Noelia Fuentes, Cristina Nevado, University of Zurich

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Kaori Fujisawa, Stefan Matile, University of Geneva

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 Markus Gantenbein, *Marcel Mayor*, University of Basel
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Patricia García Domínguez, Cristina Nevado, University of Zurich

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Giulio Gasparini, Stefan Matile, University of Geneva

Synthesis of Cyano-Substituted Diaryltetracenes from Tetraaryl[3]cumulenes [OC-126]

Przemyslaw Gawel, François Diederich, ETH Zurich

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Ori Gidron, François Diederich, ETH Zurich

Retention of Absolute Configuration in Hydrogen Atom Transfer/Cyclisation Cascade [OC-129]

Christian Gloor, Philippe Renaud, University of Bern

- Peptide-Catalyzed Stereoselective Conjugate Addition Reactions of Aldehydes to Maleimides [OC-130] Claudio Grünenfelder, *Helma Wennemers*, ETH Zurich
- Phosphoric Acid-catalyzed Desymmetrization of Bicyclic Bislactones Bearing an All Carbon Quaternary Stereogenic Center: Catalytic Enantioselective Syntheses of (-)-Rhazinilam and (-)-Leucomidine B [OC-131] Jean-Baptiste Gualtierotti, *Jieping Zhu*, EPFL Lausanne
- Cyclic Carbo-Isosteric Depsipeptides and Peptides as a Novel Class of Peptidomimetics and their Potential Biological Applications [OC-132]
 Stephanie Gueret, *Hans-Jörg Roth*, Novartis Pharma AG
- Study of Tris-(2-carboxyethyl)-phosphine oxide [OC-133]

Jihane Haoues, University of Neuchatel

Design, Synthesis and Physical Investigation of Bias-Dependant and Mechanically Driven Single Molecular Spin Switches [OC-134]

Gero Harzmann, Marcel Mayor, University of Basel

- Synthetic Studies towards Fijiolide A [OC-135] Christoph Heinz, *Nicolai Cramer*, EPFL Lausanne
- Rotational restricted and functionalized CBP derivatives as host materials for phosphorescent organic light-emitting diodes [OC-136]

Manuel Hellstern, Marcel Mayor, University of Basel

- Mechanistic insights into C-C coupling reactions mediated by Au(I)/Au(III) redox processes [OC-137]
 Manuel Hofer, *Cristina Nevado*, University of Zurich
- Ferrocene Comprising Macrocycle Towards Rotational Restricted Molecular Wires [OC-138]

Viktor Hoffmann, Marcel Mayor, University of Basel

- Screening of Chiral Phosphine-based Organocatalysts for the Asymmetric Morita-Baylis-Hillman Reaction by Mass Spectrometric Monitoring of the Back Reaction [OC-139]
 - Patrick Isenegger, Andreas Pfaltz, University of Basel
- Stabilization of open-shell graphene fragment triangulene [OC-140]

Michal Juricek, University of Basel

- Enantioselective Synthesis of Tröger's Bases via Cu(II)catalyzed Double Aza-Michael Addition [OC-141] Takuya Kamiyama, *Jan Cvengros*, ETH Zurich
- **Towards the Total Synthesis of Fidaxomicin [OC-142]** Elias Kaufmann, *Karl Gademann*, University of Basel
- Supramolecular Zippers Dispersing Single-Walled Carbon Nano-Tubes (SWCNTs) [OC-143] Guojun Ke, *Marcel Mayor*, University of Basel
- Synthesis of chiral Ruthenium-cyclopentadienyl complexes and application to hydrative cyclisation of yne-enones [OC-144]

David Kossler, Nicolai Cramer, EPFL Lausanne

- **AFM tip functionalization by in situ click reaction [OC-145]** Rakesh Kumar, *Yoko Yamakoshi*, ETH Zurich
- A Simple Method for the Alkylation of N-Heterocycles with Trialkylboranes [OC-146]
 Andrey Kuzovlev, *Philippe Renaud*, University of Bern
- Modular Synthesis, Orthogonal Functionalization and Properties of Novel Cationic [6]Helicene [OC-147] Maria Geraldine Labrador Beltran, *Jérôme Lacour*, University of Geneva
- Organocatalyzed Direct Vinylogous Double Michael Addition of Unactivated α -Angelica Lactone to Enones [OC-148]

Roman Lagoutte, Alexandre Alexakis, University of Geneva

- Pushing Corannulene to New Extremes: Synthesis of New, Curved Polycyclic Aromatic Hydrocarbons [OC-149] Samuel Lampart, *Jay Siegel*, University of Zurich
- **Triple-Channel Photosystems [OC-150]**Santiago Lascano, *Stefan Matile*, University of Geneva
- Novel 1,2,3-Triazolium Ionic Liquids For Dye-Sensitized Solar Cells [OC-151] Genevieve Lau Pui Shan, EPFL Lausanne
- Keep It Simple! Using Asymmetric Monohydrogenation to Access Chiral Building Blocks [OC-152] Charlotte Laupheimer, *Andreas Pfaltz*, University of Basel
- Direct synthesis of a magnetic Palladium-containing ordered mesoporous carbon from a biosourced precursor. Application to Suzuki couplings [OC-153] Claude Le Drian, *Jean-Michel Becht*, Université de Haute-Alsace, Mulhouse, France
- Linear Multidentate Thioether Ligands for the Synthesis of Stable Au NP's with Increased Sizes [OC-154] Mario Lehmann, *Marcel Mayor*, University of Basel
- Oligoprolines as Scaffolds for Supramolecular Systems [OC-155]

Bartosz Lewandowski, Helma Wennemers, ETH Zurich

- Synthesis of Alkynylated Heterocycles via Direct C-H Functionalization or Domino Reactions [OC-156] Yifan Li, *Jérôme Waser*, EPFL Lausanne
- Supramolecular Control over Surface Deposition of Porphyrins [OC-157]
 - Kenan Li, Marcel Mayor, University of Basel
- Catalytic Enantioselective Synthesis and Utility of α-Quaternary Lactams [OC-158]

 Marc Liniger, *Brian M. Stoltz*, California Institute of Technology

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Michael Umberto Lüscher, Jeffrey W. Bode, ETH Zurich

Preparation of chiral functionalized magnetite nanoparticle for catalytic purposes [OC-160]

Olimpia Mamula Steiner, School of Engineering and Architecture of Fribourg

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William Maupillier, Reinhard Neier, University of Neuchatel

Anion-π Interactions in Organocatalysis [OC-162] Jadwiga Gajewy, *Stefan Matile*, University of Geneva

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Jovana Milic, François Diederich, ETH Zurich

Palladium-Catalyzed Oxy-Alkynylation of Olefins [OC-164] Ugo Orcel, *Jérôme Waser*, EPFL Lausanne

Functionalized Low-Density Lipoprotein Nanoparticle as NIR Imaging Probe for Atherosclerosis with MMP2-specific Ligand Site [OC-165] Sean Oriana, Yoko Yamakoshi, ETH Zurich

Access to β-Lactams by Enantioselective Palladium (0)-Catalyzed C(sp³)-H Alkylation [OC-166]
Julia Pedroni, *Nicolai Cramer*, EPFL Lausanne

Rh^{III}-Catalyzed C-H Activation Rapid Access to Complex Organic Molecules [OC-167]

Van-Manh PHAM, Nicolai Cramer, EPFL Lausanne

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Ewa Pietrasiak, Antonio Togni, ETH Zurich

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Lucas Prieto, Felix Zelder, University of Zurich

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Sophie Racine, Jérôme Waser, EPFL Lausanne

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Tristan Reekie, François Diederich, ETH Zurich

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Peter Ribar, University of Basel

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Michel Rickhaus, Marcel Mayor, University of Basel

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Italo Sanhueza, ETH Zurich, Franziska Schoenebeck, RWTH Aachen

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Geoffrey Schwertz, François Diederich, ETH Zurich

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Shuo Tong, Jieping Zhu, EPFL Lausanne

Fluorescent Amphiphilic Push-Pull Oligothiophenes as Planarizable and Polarizable Membrane Probes [OC-181]

Quentin Verolet, Stefan Matile, University of Geneva

Synthesis of functionalized polyether macrocycles [OC-182] Mahesh Vishe, *Jérôme Lacour*, University of Geneva

Pd(0)-Catalyzed Enantioselective Synthesis of 1,5-Enynes. [OC-183]

Maria Victoria Vita, Jérôme Waser, EPFL Lausanne

Hierarchical self-assembly of nucleotide-appended oligopyrenotides into defined supramolecular objects [OC-184] Yuliia Vyborna, *Robert Häner*, University of Bern

N-aminoacridinium cations: central building blocks for the synthesis of unprotected aziridines and pH-sensitive dyes synthesis [OC-185]

Antoine Wallabregue, Jérôme Lacour, University of Geneva

Towards a Perylene-Based Cyclophane with Charge-Transfer Capability [OC-186]

Kevin Weiland, Marcel Mayor, University of Basel

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Baihua Ye, Nicolai Cramer, EPFL Lausanne

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Ultra-Broadband Multidimensional Electronic Spectroscopy Setup [PC-101]

Andre Al Haddad, Majed Chergui, EPFL Lausanne

High resolution THz spectroscopy between 0.8 and 3 THz with a Synchrotron source and a Bruker interferometer. [PC-102]

Sieghard Albert, ETH Zurich, *Alexander Wokaun*, Paul Scherrer Institute, Villigen

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Pitt Allmendinger, Frédéric Merkt, ETH Zurich

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 - Franziska Balmer, Samuel Leutwyler, University of Bern
- Multichannel quantum defect theory (MQDT) assisted spectroscopy of H+, through the Rydberg spectrum of H,. [PC-106]
 - Maximilian Beyer, Frédéric Merkt, ETH Zurich
- Energytransfer of Eu²⁺ in SrAl₂O₄ codoped with Dy³⁺ [PC-107]
 - Jakob Bierwagen, Hans Hagemann, University of Geneva
- **Excited State Photophysics of Jet-Cooled 2-Aminopurine** and 9-Methyl-2-Aminopurine [PC-108]
 - Susan Blaser, Samuel Leutwyler, University of Bern
- High Resolution Analysis of the FTIR spectra and quantum dynamics of CHF₃: The $2v_4$ (A₁/E) Band [PC-109] Irina Bolotova, Martin Quack, ETH Zurich
- Effect of Ba and K addition and controlled spatial deposition of Rh in Rh/Al,O, catalysts for CO, hydrogenation
 - Robert Büchel, Alfons Baiker, ETH Zurich
- Plasmon tuning of gold nanoparticles array for surface enhanced Raman scattering [PC-111]
 - Mahshid Chekini, Thomas Bürgi, University of Geneva
- **Solvation Dynamics Around Photo-excited Transition Metal** Complexes: A Molecular Dynamics Approach [PC-112] Akshaya Das, Markus Meuwly, University of Basel
- **Structure of n-Alkanes [PC-113]**
 - Takuya Den, Samuel Leutwyler, University of Bern
- Ultrafast excited-state dynamics of flavonol anion: no intermolecular proton transfer [PC-114]
 - Bogdan Dereka, Eric Vauthey, University of Geneva
- Signal Enhancement & Artifacts Suppression in Vibrational Circular Dichorism Spectroscopy with Femtosecond Lasers [PC-115]
 - Biplab Dutta, Jan Helbing, University of Zurich
- **Controlled Chemistry using Cold Atomic or Molecular Ions** and Ultracold Atoms in Hybrid Traps [PC-116] Pascal Eberle, Stefan Willitsch, University of Basel
- Photo-induced fibril formation [PC-117]
 - Lukas Frey, Peter Hamm, University of Zurich
- Photoprotection of an oxazine dye by quencher amino acids in model peptides [PC-118]
 - Alexandre Fürstenberg, University of Geneva
- Observation and theory of electric-dipole-forbidden infrared transitions in cold molecular ions [PC-119]
 - Matthias Germann, Stefan Willitsch, University of Basel
- Nanoparticle polyelectrolyte composites investigated by ATR-IR spectroscopy: Enhanced IR absortion and electron transfer upon visible light illumination [PC-120] Harekrishna Ghosh, University of Geneva
- Quantifying a Molecular Orbital's Character using **Resonant Photoemission [PC-121]**
 - Jakob Grilj, EPFL Lausanne, Markus Gühr, Stanford University
- First rotational interval of para H₂⁺ by Rydberg spectroscopy of H, in the range of 0.3-7 THz [PC-122]

Christa Haase, Frédéric Merkt, ETH Zurich

- High-Resolution Absorption Spectroscopy in the Vacuum-**Ultraviolet using Modulation Techniques [PC-123]** U. Hollenstein, Frédéric Merkt, ETH Zurich
- Excited-state dynamics of chiral molecules at the liquidliquid interface [PC-124]
 - Cho-Shuen Hsieh, Eric Vauthey, University of Geneva
- Mass Accommodation Coefficients and Evaporation Rates of H₂O, HCl and HNO₃ on Atmospheric Ices in the Range 170 to 210 K [PC-125]
 - Riccardo Iannarelli, Michel J. Rossi, Paul Scherrer Institute, Villigen
- Exciplex Formation in Bimolecular Photoinduced Electron-Transfer Investigated by Ultrafast Time-Resolved Infrared Spectroscopy [PC-126]
 - Marius Koch, Eric Vauthey, University of Geneva
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 - Philipp Kowalewski, Samuel Leutwyler, University of Bern
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 - Peter Kraus, Hans Jakob Wörner, ETH Zurich
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 - Peter Kraus, Hans Jakob Wörner, ETH Zurich
- Sub-70 Femtoseconds Time-resolved Fluorescence Made Easy [PC-130]
 - Romain Letrun, Eric Vauthey, University of Geneva
- Nanostructured Metallic Aerogels: High Performance **Electroctrocatalysts for Fuel Cell Reactions [PC-131]** Wei Liu, Technische Universität Dresden, Germany
- Pressure induced transformations in molecular crystals [PC-132]
 - Piero Macchi, University of Bern
- Raman Optical Activity (ROA) study on the conformation of (L)- ascorbic acid in aqueous solution [PC-133] Martin Magg, *Thomas Bürgi*, University of Geneva
- A Jet-CRDS Investigation of the v2+2v3 band of ¹³CH₄ [PC-134]
 - Carine Manca Tanner, Martin Quack, ETH Zurich
- Rational design of technical dawsonite-based sorbents for post-combustion CO, capture [PC-135] Oliver Martin, Javier Pérez-Ramírez, ETH Zurich
- Development of scanning electrochemical microscopy methods for the examination of copper(I) complexes in dye sensitized solar cells [PC-136]
 - Colin Martin, Edwin C. Constable, University of Basel
- Steps towards molecular parity violation: Population transfer experiments and absolute frequencies and quadrupole splittings of the lowest ro-vibrational levels (J = 1) of v1, $v3\pm 1$, 2v40 and $2v4\pm 2$ in NH, [PC-138]
 - Eduard Miloglyadov, Martin Quack, ETH Zurich
- Cold molecular ions on a chip [PC-139]
 - Arezoo Mokhberi, Stefan Willitsch, University of Basel
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 - Roberto Monni, Majed Chergui, EPFL Lausanne

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Sandra Mosquera Vazquez, Eric Vauthey, University of Geneva

A table-top high-harmonic-generation-based source for valence/core level photoelectron spectroscopy in liquid samples [PC-142]

Jose Ojeda, Majed Chergui, EPFL Lausanne

Ultrafast spectroscopic investigation of carrier dynamics in Dye sensitized and perovskite based photovoltaics [PC-143]

Arun Aby Paraecattil, Jacques-E. Moser, EPFL Lausanne

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Khrystyna Regeta, Michael Allan, University of Fribourg

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Arnulf Rosspeintner, Eric Vauthey, University of Geneva

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Heiner Sassmannshausen, Frédéric Merkt, ETH Zurich

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Janne Savolainen, Peter Hamm, University of Zurich

Computational Study of Spectroscopic Properties of Different Borohydride Species [PC-148]

Daniel Sethio, Hans Hagemann, University of Geneva

Disorder-Suppressed Vibrational Relaxation in Vapor-Deposited High-Density Amorphous Ice [PC-149] Andrey Shalit, *Peter Hamm*, University of Zurich

Reversible Isotope Exchange Reactions in Ca(BH₄)₂ [PC-150]

Manish Sharma, Hans Hagemann, University of Geneva

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Luca Siffert, Samuel Leutwyler, University of Bern

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Erik Stronks, University of Zurich

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Maria Trachsel, Samuel Leutwyler, University of Bern

The Solvated Carbon-Fluorine Bond in Water Investigated by 2D IR spectroscopy [PC-155]

Halina Tran, Peter Hamm, University of Zurich

Alignment effects in the dissociative chemisorption of methane: the role of vibrational symmetry [PC-156] Maarten van Reijzen, *Rainer Beck*, EPFL Lausanne

A high-flux femtosecond XUV beamline for time-resolved photoelectron spectroscopy [PC-157]

Aaron von Conta, Hans Jakob Wörner, ETH Zurich

Imaging Electronic Wave Packets Through Electron Rescattering and Holography [PC-158]

Samuel Walt, Hans Jakob Wörner, ETH Zurich

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Jun Xu, University of Zurich

Excited-state dynamics of multichromophoric arrays [PC-161]

Oleksandr Yushchenko, Eric Vauthey, University of Geneva

Continuous trap loading of Rydberg atoms and molecules using overlaid electric and magnetic traps [PC-162] Matija Zesko, *Frédéric Merkt*, ETH Zurich

Placing Nanosheets on Graphene [PC-163]

Zhikun Zheng, A. Dieter Schlüter, ETH Zurich

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Ganna Berezovska, Albert-Ludwigs University of Freiburg, *Markus Meuwly*, University of Basel

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Formation of supramolecular polymers by chrysene oligomers [PI-031]

Caroline Bösch, Robert Häner, University of Bern

Microenvironment of the Interior of Dendronized Polymers [PI-032]

Chiara Gstrein, A. Dieter Schlüter, ETH Zurich

Poleable nanoparticles as fillers towards non-linear optically active actuators [PI-033]

Yee Song Ko, EPFL Lausanne, Frank Nüesch, EMPA Dübendorf

Functional Surface Engineering by Insertion of Membrane Protein into Solid-Supported Polymer Membranes [PI-034]

Justyna Kowal, Wolfgang Meier, University of Basel

Importance of particulate organic matter in singlet oxygen mediated photochemistry [PI-101]

Elena Appiani, Kristopher McNeill, ETH Zurich

Superficial Doping Allows Growth of Silicone Nanostructures on Hydroxyl-free Substrates [PI-102] Georg Artus, Stefan Seeger, University of Zurich

Towards 2D-Polymers: Synthesis of a Rotor-shaped Monomer [PI-103]

Simon T. Cerqua, A. Dieter Schlüter, ETH Zurich

Tripeptides as Additives for the Controlled Formation of Palladium Nanoparticles [PI-104]

Stefano Corrà, Helma Wennemers, ETH Zurich

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Virginia Crivelli, Christine Wandrey, EPFL Lausanne

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Bernd Deffner, A. Dieter Schlüter, ETH Zurich

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Simon Dünki, EPFL Lausanne, *Dorina Opris, EMPA Dübendorf*

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Michael Felber, Roger Alberto, University of Zurich

- Enzyme-catalyzed Atom Transfer Radical Polymerization of Heterocyclic Aromatic Vinyl Compounds [PI-109] Csaba Fodor, *Nico Bruns*, University of Fribourg
- Nano-Handling of Individual Dendronized Polymers [PI-110]

Lucie Grebikova, Michal Borkovec, University of Geneva

- **Self-Assembly of Magnetic Janus Dumbbells [PI-111]**Florian Guignard, *Marco Lattuada*, University of Fribourg
- **Hybrid bio-responsive nanocapsules [PI-112]**Dawid Kedracki, *Corinne Vebert*, University of Geneva
- Gram-Scale Synthesis of Organic Two-Dimensional Polymer Crystals and Exfoliation into Nanometer-Thin Sheets [PI-113]

Max J. Kory, A. Dieter Schlüter, ETH Zurich

- Enzyme Immobilization with Dendronized Polymer-Enzyme Conjugates for Localized Cascade Reactions [PI-114] Andreas Küchler, *Peter Walde*, ETH Zurich
- pH-dependent Degradation Kinetics of Polylactic Acid [PI-115]

Stefano Lazzari, Massimo Morbidelli, ETH Zurich

Synthesis of oriented nano-wires on a microfluidic platform [PI-116]

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