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Chemische
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SSC
Société Suisse
de Chimie

SCS
Swiss Chemical
Society

DIVISIONS:
ANALYTICAL SCIENCES
MEDICINAL CHEMISTRY
& CHEMICAL BIOLOGY
FUNDAMENTAL RESEARCH
POLYMERS, COLLOIDS
& INTERFACES

DIVISIONEN:
ANALYTISCHE WISSENSCHAFTEN
MEDIZINISCHE CHEMIE
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GRUNDLAGENFORSCHUNG
POLYMERE, KOLLOIDE
& GRENZFLÄCHEN

DIVISIONS:
SCIENCES ANALYTIQUES
CHIMIE THERAPEUTIQUE
& CHIMIE BIOLOGIQUE
RECHERCHE FONDAMENTALE
POLYMERES, COLLOÏDES
& INTERFACES

Fall Meeting 2013

Herbstversammlung 2013

Assemblée d'automne 2013

Friday, September 6, 2013

Freitag, 6. September 2013

Vendredi, 6 septembre 2013



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Ecole Polytechnique Fédérale de Lausanne
Centre Est

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Information

No admission fee will be charged to SCS members. SCS members **must identify themselves** at the registration desk with their **membership card**.

Non-members of the SCS will be charged a 50 CHF admission fee, which will provide access to the conferences, poster sessions, coffee breaks and lunch.

Lunch: Sandwiches, pastries and drinks will be offered in the vicinity of the poster session. A cafeteria and a restaurant are located next to the meeting venues.

Coffee breaks: Coffee and drinks will be available until 10.30 in the morning and a coffee break will be organized between 17.00 and 17.15, before the Plenary Session II.

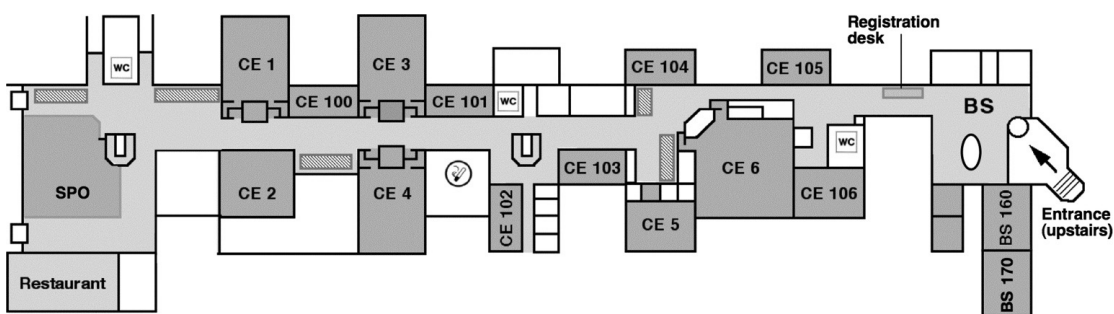
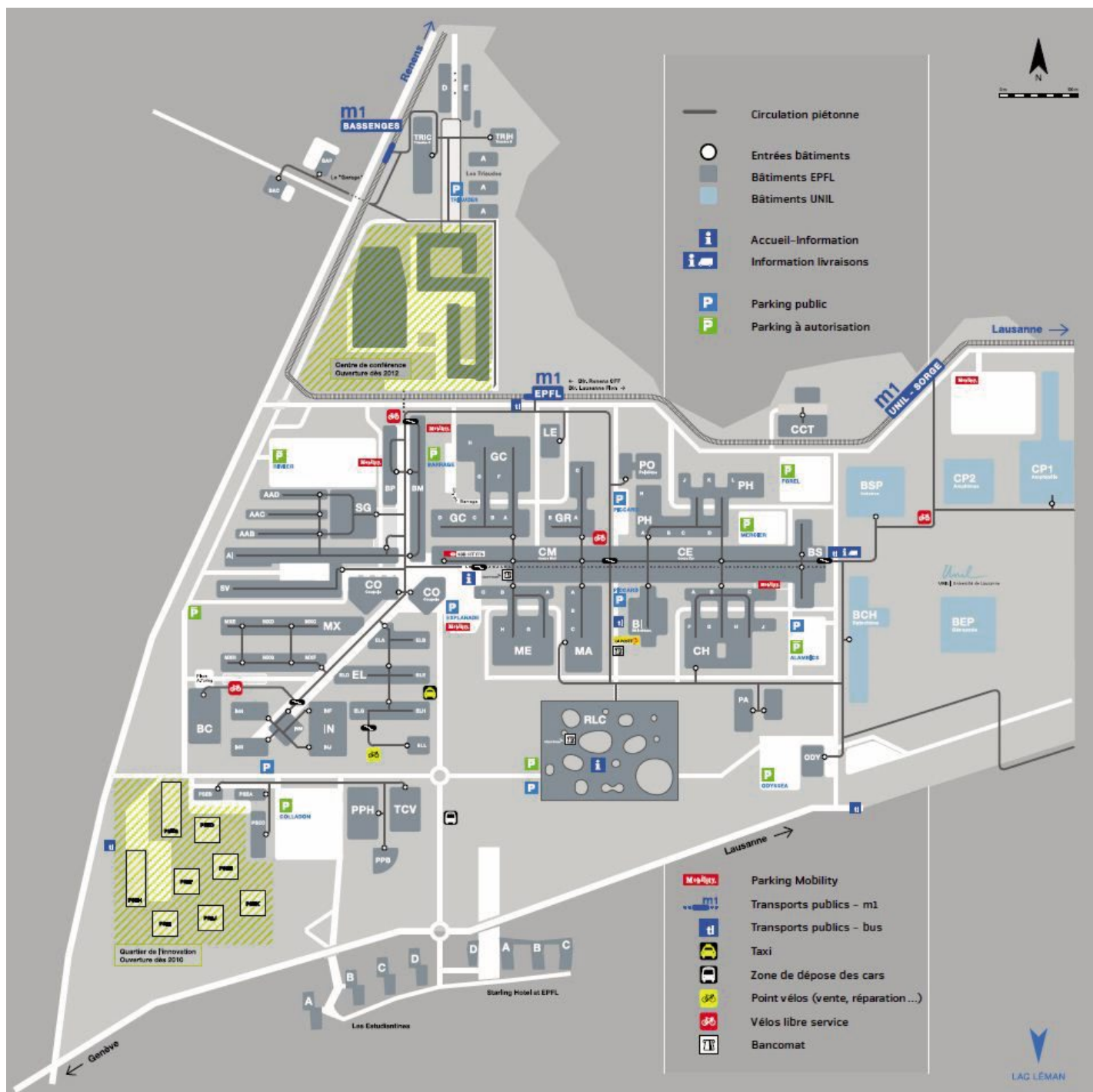
Transportation

By train: Only limited parking space will be available on the campus of the Ecole Polytechnique Fédérale de Lausanne. Hence, travelling by train is recommended. EPFL campus can be easily reached by metro (tramway), either from Lausanne or Renens train stations. Travelers arriving at Lausanne can continue their journey with the metro (m2 line from the train station to Flon, m1 line from Flon to Unil-Sorge). From Renens station, the trip by metro (m1 line) to *UNIL-Sorge* stop is 7 min. 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 parkings of the building *Odyssey* and of *the Rolex Learning Center* (see EPFL campus map here below). One-day parking permits will be sold on the parking lot and at the entrance of the BS building for CHF 5.–.

Train Timetable

Train from	Morning			Evening			Train to
	Departure	Arrival Lausanne	Arrival Renens	Departure Renens	Departure Lausanne	Arrival	
Basel	07.04	09.15	09.25	19.10		21.53	Basel
Bern	08.04	09.10	09.25	19.04	19.20	20.26	Bern
Fribourg	08.26	09.10	09.25	19.04	19.20	20.03	Fribourg
Geneva	08.33	09.12	09.25	18.56		19.39	Geneva
Neuchâtel	08.34	09.15	09.25	19.10		20.22	Neuchâtel
Zürich	07.04	09.15	09.25	19.04	19.20	21.28	Zürich



EPFL Campus

The meeting will be held on the first floor of 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 yellow signs.

Detailed Map of Lecture Halls

Opening Ceremony, Plenary Sessions	CE 6		
Analytical Sciences	CE 2 (Lectures)	CE 100 (Posters)	
Catalysis Science & Engineering	CE 1 (Lectures)	CE 104 (Posters)	
Computational Chemistry	CE 105 (Lectures)	CE 102 (Posters)	
Inorganic & Coordination Chemistry	CE 3 (Lectures)	CE 103 (Posters)	
Medicinal Chemistry & Chemical Biology	CE 6 (Lectures)	SPO (Posters)	
Organic Chemistry	CE 5 (Lectures, A)	CE 106 (Lectures, B)	SPO (Posters)
Physical Chemistry	CE 4 (Lectures)	CE 101 (Posters)	
Polymers, Colloids & Interfaces	BS 160 (Lectures)	BS 170 (Posters)	

Award Program

At the Fall Meeting, the best presentations (oral and poster) will be awarded a prize sponsored by DSM (posters) and by the Metrohm Foundation (oral presentations).



The prizes consist of a cash contribution, and a travel voucher to attend an international conference. In addition, the winners in each session will be invited to present their research in the Laureates issue of CHIMIA.

The members of the Award Jury are listed at the Fall Meeting website (www.scg.ch/fallmeeting). The Award Ceremony marks the end of the Fall Meeting (Plenary Session II).

Sponsors

The meeting organizers gratefully acknowledge the generous support of its sponsors. See below for the names and logos of the sponsors.



Kontaktgruppe für Forschungsfragen (KGF)



Swiss Academy of Sciences
Akademie der Naturwissenschaften
Accademia di scienze naturali
Académie des sciences naturelles

**Commercial Exhibition**

A number of exhibitors will be presenting their products and services at the Fall Meeting. The Commercial Exhibition will take place in the main hall of CE building from 9.30 to 17.30. See below for the company names and logos.



GENERAL
MICROTECHNOLOGY
& PHOTONICS

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	Analytical Sciences	Catalysis Science & Engineering	Computational Chemistry	Inorganic & Coordination Chemistry	Organic Chemistry Sessions A / B	Physical Chemistry	Medicinal Chemistry & Chemical Biology	Polymers, Colloids & Interfaces
10	Plenary Session I, CE 6 Opening address Grammatikakis Neumann Lecture, U. Pischel (University of Huelva) Sandmeyer Lecture, P. Steffanut and S. Bellemin (Clariant Group R&D, CNRS-Université de Strasbourg)							
11	Gen. Ass., CE 2 Session I, CE 2 Invited lecture AS01 Talks AS02-05	Session I, CE 1 KGF SII Lecture CSE01 Invited Lecture CSE02 Talks CSE04-07	Session I, CE 105 Talks CC01-08	Session I, CE 3 Invited Lecture IC01 Talks IC02-06	Session I, CE 5/CE 106 KGF II Lecture OC002 A, Talks OC004-011 B, Talks OC018-024	Session I, CE 4 Talks PC01-07 Poster talks PC08-12	Session I, CE 6 KGF SII Lecture MC001 Talks MC002-007	Session I, BS 160 Invited Lecture PCI01 Talks PCI03-07
12	General Assembly, Division of Fundamental Research, CE 5							
13	Lunch Poster Session, 13.15-14.30 Commercial Exhibition, 09.30-17.30							
14	General Assembly of the SCS, CE 6							
15	Session II, CE 2 Talks AS06-13	Session II, CE 1 Invited Lecture CSE03 Talks CSE08-13	Session II, CE 105 Talks CC09-16	Session II, CE 3 Talks IC07-14	Session II, CE 5/CE 106 Invited Lecture OC001 Invited Lecture OC003 A, Talks OC012-017 B, Talks OC25-30	Session II, CE 4 Talks PC13-20	Session II, CE 6 Talks MC008-016	Session II, BS 160 Invited Lecture PCI02 Talks PCI08-12
16	General Assembly of the SCS, CE 6							
17	Plenary Session II, CE 6 KGF Distinguished Industrial Investigator Lecture, K. Müller (F. Hoffmann-La Roche AG), 17.15-17.50 Awards for best poster and oral presentations sponsored by DSM and the Metrohm Foundation, 17.50-18.10							
18	General Assembly of the SCS, CE 6							

Session Program

PLENARY SESSIONS

Plenary Session I (CE 6)

- 09.45–11.00** **Opening Ceremony**
EPFL, CE 6
Opening address
Thomas Rizzo
Dean of the School of Basic Sciences, EPFL
- Grammaticakis-Neumann Lecture**
Chair: **E. Peter Kündig** (SCS President)
- Uwe Pischel**, University of Huelva
Molecular Switches with Logic Functions
Abstract P1
- Sandmeyer Lecture**
Chair: **E. Peter Kündig** (SCS President)
- Pascal Steffanut^a and Stéphane Bellemin-Laponnaz^b**, ^aClariant Group R&D, ^bCNRS-Université de Strasbourg
Ti(IV) and Zr(IV) N-heterocyclic carbene complexes: synthesis, reactivity and use of them in the controlled ring-opening polymerization of rac-lactide and trimethylene carbonate
Abstract P2

General Assemblies of the Divisions

- 11.00–11.15** **Division of Analytical Sciences (CE 2)**
Chair: **Gérard Hopfgartner** (University of Geneva)
- 13.00–13.15** **Division of Fundamental Research (CE 5)**
Chair: **Philippe Renaud** (University of Bern)
- Division of Medicinal Chemistry & Chemical Biology (CE 6)**
Chair: **Karl-Heinz Altmann** (ETH Zürich)
- Division of Polymers, Colloids & Interfaces (BS 160)**
Chair: **Bettina Steinmann** (3D Systems)
- 13.45–14.30** **General Assembly of the Swiss Young Chemists' Association (CE 5)**
Chair: **Lars Ruddigkeit** (University of Bern)

General Assembly of the SCS (CE 6)

- 14.30–15.00** **General Assembly of the Swiss Chemical Society**
Chair: **E. Peter Kündig** (SCS President)

PLENARY SESSION II (CE 6)

- 17.15–17.50** **Lecture of the KGF Distinguished Industrial Investigator Award Laureate 2013**
Chair: **R. Naef** (Kontaktgruppe für Forschungsfragen), **E. P. Kündig** (SCS President)
- Klaus Müller**
F. Hoffmann-La Roche AG, Basel
30 Years at the Interface between Science and Technology
Abstract P3
- 17.50–18.10** **Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation**
Chair: **E. P. Kündig** (SCS President)

PARALLEL SESSIONS

Analytical Sciences

- 11.00–11.15** **General Assembly of the Division**
Chair: **Gérard Hopfgartner** (University of Geneva)
- 11.15–13.00** **Session I (CE 2)**
Chair: **Stefan Schürch** (University of Bern)
Abstracts AS01–AS05
- 11.15** **Invited lecture**
Hubert Girault, EPF Lausanne
ESTASI
Abstract AS01
- 12.00** **Daniel Frick**, C. Giesen, T. Hemmerle, D. Neri, B. Bodenmiller, D. Günther, ETH Zürich and University of Zürich
Evaluation of Standards for Quantitative Tissue Imaging by LA-ICP-MS (AS02)
- 12.15** **F. Kálmán**, M. E. Pfeifer, D. Prim, **Miriam Goyder**, HES-SO Valais
Mass Spectrometry Based Disulfide Assignment in Venom Proteins (AS03)
- 12.30** **Xue Li**, R. Zenobi, ETH Zürich and Shanghai University
Development of an online solid phase extraction system using polyetheretherketone tubing coupled to ion trap tandem mass spectrometry (AS04)

- 12.45** **Thomas B. Jensen**, J.-P. Bourgeois, J. J. Jodry, EIA Fribourg and Metalor Technologies SA
Microwave Plasma – Atomic Emission Spectroscopy: a novel technology for the analysis of impurities in gold (AS05)
- 13.00–14.30** **Poster session (CE 100)**
Abstracts AS14–AS54
- 15.00–17.00** **Session II (CE 2)**
Chair: **Hanspeter Andres** (METAS, Bern-Wabern)
Abstracts AS06–AS13
- 15.00** **Luca Fornelli**, U. A. Laskay, A. N. Kozhinov, K. Srzentić, D. Ayoub, Y. O. Tsybin, EPF Lausanne
Structural analysis of monoclonal antibodies by top-down and middle-down mass spectrometry (AS06)
- 15.15** **Denis Prim**, V. Cosandey, F. Rebeaud, M. E. Pfeifer, HES-SO Valais
Advances in azide-alkyne cycloaddition (click-chemistry) based manufacturing of molecular diagnostic peptide microarrays (AS07)
- 15.30** **Fanny Widjaja**, V. Frankevich, K. Barylyuk, Z. Yang, R. Zenobi, ETH Zürich
Fluorescence Resonance Energy Transfer of Gas-Phase Ions under Ambient Conditions (AS08)
- 15.45** **Kristina Srzentić**, U. A. Laskay, Y. O. Tsybin, EPF Lausanne
Utility of chemical agents for high-throughput protein characterization (AS09)
- 16.00** A. M. Castillo, J. Wist, L. Patiny, **Andrés Bernal**, National University of Colombia and EPF Lausanne
A Comparison of NMR Predictors Using Binary Tree Similarity of Spectra (AS10)
- 16.15** **Konstantin O. Zhurov**, A. N. Kozhinov, Y. O. Tsybin, EPF Lausanne
Fossil fuel analysis via high resolution mass spectrometry (AS11)
- 16.30** **Grégoire Bonvin**, S. Rudaz, J. Schappler, University of Geneva and University of Lausanne
Analysis of acidic compounds by CE in negative ESI-MS with organic solvents (AS12)
- 16.45** **Caroline Münsterer**, L. Wacker, B. Hattendorf, M. Christl, J. Koch, R. Dietiker, H.-A. Synal, D. Günther, ETH Zürich
¹⁴C analysis of carbonates at high spatial resolution by the coupling of Laser Ablation with AMS (AS13)

Catalysis Science and Engineering

Session Endowment: Clariant

- 11.10–13.00** **Session I (CE 1)**
Abstracts CSE01, CSE02, CSE04–CSE07
- 11.00** **Lecture of the KGF Senior Industrial Investigator Award Laureate 2013**
Chair: **Xile Hu** (EPF Lausanne)
- Werner Bonrath**
DSM Nutritional products, Basel
New trends in (heterogeneous) catalysis in the fine chemical industry
Abstract CSE01
- 11.30** **Invited lecture**
Chair: **Xile Hu** (EPF Lausanne)
- Gerhard Mestl**
Clariant Produkte GmbH
Multicomponent Catalysts for Oxidation of Propane to Acrylic Acid developed by combinatorial approach
Abstract CSE02
- Oral Communications**
Chair: **Gerhard Mestl** (Clariant Produkte GmbH)
- 12.00** **Roche M. Walliser**, R. Toth, F. Boudoire, A. Braun, E. C. Constable, University of Basel and EMPA Dübendorf
'Green Energy' by solar water splitting (CSE04)
- 12.15** **Karol Furman**, D. Baudoin, F. Ribeiro, C. Copéret, ETH Zürich and Purdue University
Ruthenium nanoparticle supported on hydrophobic silica: a change on surface properties and reactivity (CSE05)
- 12.30** **Xiaoying Xu**, S. M. Rummelt, F. L. Morel, M. Wörle, M. Ranocchiari, J. A. van Bokhoven, ETH Zürich and PSI Villigen
Steric Control at the Active Site in Organocatalysis by Phosphine Metal-Organic Frameworks (CSE06)
- 12.45** **Gianvito Vilé**, L. Floryan, J. Pérez-Ramírez, ETH Zürich
Selective CeO₂-based catalysts for liquid-phase hydrogenation of triple bonds in polyunsaturated and polyfunctionalized substrates (CSE07)
- 13.00–14.30** **Poster session (CE 104)**
Abstracts CSE14–CSE59
- 15.00–17.00** **Session II (CE 1)**
Abstracts CSE03, CSE08–CSE13

- 15.00** *Invited lecture*
Chair: **Christophe Copéret** (ETH Zürich)
- Ib Chorkendorff**
Danish Technical University, Denmark
New electro-catalyst alloys for the Oxygen Reduction Reaction (ORR) and Hydrogen Peroxide production
Abstract CSE03
- Oral Communications*
Chair: **Ib Chorkendorff** (Danish Technical University)
- 15.30** **Tobias Keller**, S. Isabetini, J. Pérez-Ramírez, ETH Zürich
Reinventing zeolite base catalysis: Less is more (CSE08)
- 15.45** **Rocio Micaela Crespo-Quesada**, A. Prestianni, R. Cortese, L. Kiwi-Minsker, D. Duca, EPF Lausanne and Università degli Studi di Palermo
When DFT Calculations Meet Experimental Results: Understanding the Structure Sensitivity of Alkyne Hydrogenations on Pd nanoparticles (CSE09)
- 16.00** **Amaia Beloqui Redondo**, M. A. Brown, J. A. van Bokhoven, ETH Zürich and PSI Villigen
Performance of a Au/Al₂O₃ catalyst in the decomposition of formic acid (CSE10)
- 16.15** **Artur Yarulin**, I. Yuranov, F. Cárdenas-Lizana, L. Kiwi-Minsker, EPF Lausanne
Activity and Selectivity of Pd Catalyst in Liquid-Phase Alkynol Hydrogenation: Effect of Particle Size and Modification with the Second Metal (CSE11)
- 16.30** **Emiliana Fabbri**, R. Kötz, T. J. Schmidt, PSI Villigen
Advanced cathode materials based on Pt-oxide systems for application in polymer electrolyte fuel cells (PEFCs) (CSE12)
- 16.45** **Sylvain Keav**, Y. Lu, A. E. Maegli, S. K. Matam, A. Heel, A. Weidenkaff, D. Ferri, EMPA Dübendorf and PSI Villigen
Deactivation of a commercial honeycomb noble metal-based CO oxidation catalyst by Cr-containing species (CSE13)
- 11.15** **Miroslav Sulc**, J. Vaníček, EPF Lausanne
Relation of exact Gaussian basis methods to the dephasing representation: twelve methods for computing time-resolved electronic spectra (CC02)
- 11.30** **Eric Brémond**, C. Corminboeuf, EPF Lausanne
Exciton Coupling in Organic Electronic Assemblies: a Challenge for DFT Approximations (CC03)
- 11.45** **Harry Ramanantoanina**, C. Daul, University of Fribourg
Ligand Field Density Functional Theory Approach for Two-Open Shell f and d electrons (CC04)
- 12.00** **Gloria Capano**, T. J. Penfold, U. Röthlisberger, M. Chergui, I. Tavernelli, EPF Lausanne
Solvent effects and nonadiabatic dynamics of [Cu(dmp)₂]⁺ (CC05)
- 12.15** **Sapana V. Shedge**, T. A. Wesolowski, University of Geneva
Evaluation of solvatochromic shift using the average electron density of solvent (CC06)
- 12.30** **Juan Carlos Castro-Palacio**, T. Nagy, M. Meuwly, University of Basel
The Reactive Collision and Final State Analysis of NO and O Reaction (CC07)
- 12.45** **Shuguang Yuan**, H. Vogel, S. Filipek, EPF Lausanne
The Role of Water and Sodium Ions in m-Opioid Receptor Activation (CC08)
- 13.00–14.30** **Poster session (CE 102)**
Abstracts CC17–CC37
- 15.00–17.00** **Session II (CE 105)**
Chair: **Jiri Vaníček** (EPF Lausanne)
Abstracts CC09–CC16
- 15.00** **Izabela Czekaj**, PSI Villigen
DFT studies of lignin vibrational structure (CC09)
- 15.15** **Florent Hédin**, M. Meuwly, University of Basel
Spatial averaging: enhancement of the sampling of the configuration space for atomic clusters and biomolecules (CC10)
- 15.30** **Jérôme F. Gontier**, C. Corminboeuf, EPF Lausanne
Application of the Chemical Hamiltonian to Zeroth-order Wavefunction and Energy for Intramolecular Symmetry-Adapted Perturbation Theory (CC11)
- 15.45** **Alberto Hernando**, J. Vaníček, EPF Lausanne
A novel adaptive mesh method for diagonalizing multidimensional quantum Hamiltonians (CC12)

Computational Chemistry

- 11.00–13.00** **Session I (CE 105)**
Chair: **Clémence Corminboeuf** (EPF Lausanne)
Abstracts CC01–CC08

- 11.00** **Marie Humbert-Droz**, P. Oulevey, L. M. Lawson Daku, H. Hagemann, T. Buergi, University of Geneva
Modelisation of the Raman Optical Activity of solvated 'Lambda'-Rhodium-tris-ethylenediamine (CC01)

- 16.00** **Tibor Nagy**, M. Soloviov, M. Meuwly, University of Basel
Optimal parameterization of force fields for thermal dynamics (CC13)
- 16.15** **Lars Ruddigkeit**, L. C. Blum, J.-L. Reymond, University of Bern
Ligand-Based Virtual Screening on Billions of Molecules (CC14)
- 16.30** **Negar Ashari Astani**, E. Brunk, B. Curchod, I. Tavernelli, M. Grätzel, U. Röthlisberger, EPF Lausanne
Classical Molecular Dynamics Simulation of Porphyrin-Based Dye-Sensitized Solar Cells (CC15)
- 16.45** **Marius Wehrle**, J. Vaníček, EPF Lausanne
On-the-fly wave-packet propagation: Evaluation of vibrationally resolved electronic spectra of large systems (CC16)

Inorganic and Coordination Chemistry

Session Endowment: KGF

- 11.00–13.00** **Session I (CE 3)**
Chair: **Thomas Ward** (University of Basel)
Abstracts IC01–IC06
- 11.00** **Invited lecture**
Joost Reek, University of Amsterdam, Netherlands
Supramolecular strategies in Transition metal catalysis
Abstract IC01
- 11.45** M. Nielsen, E. Alberico, **Angèle Monney**, H. Junge, M. Beller, Leibniz-Institut für Katalyse e. V., Rostock
Catalytic H₂ production from biomass-relevant alcohols under mild conditions (IC02)
- 12.00** **Marc Walter**, K. Kravchynk, L. Protesescu, M. I. Bodnarchul, F. Krumreich, M. Yarema, C. Guntlin, M. V. Kovalenko, ETH Zürich and EMPA Dübendorf
Highly Monodisperse Tin Nanocrystals as Anode Material in High-Performance Lithium-ion batteries (IC03)
- 12.15** **Federico Giannini**, J. Furrer, G. Süss-Fink, University of Bern and University of Neuchâtel
Trithiolato-bridged Dinuclear p-cymene Ruthenium complexes: A Study of their High in vitro Anticancer Activity (IC04)
- 12.30** **Lydia Paul**, J. Furrer, B. Therrien, University of Bern and University of Neuchâtel
Reactivity of hexaruthenium assemblies towards nucleotides and DNA (IC05)
- 12.45** **Yvens Chérémond**, K. M. Fromm, University of Fribourg

New metal Aryloxide complexes as ceramic precursors and Initiators for Ring-Opening Polymerization (IC06)

13.00–14.30 **Poster session (CE103)**
Abstracts IC15–IC72

15.00–17.00 **Session II (CE 3)**
Chair: *Kay Severin* (EPF Lausanne)
Abstracts IC07–IC14

15.00 **Aleix Comas-Vives**, M. P. Conley, A. J. Rossini, A. Lesage, L. Emsley, C. Copéret, ETH Zürich and University of Lyon
¹¹⁹Sn Surface Enhanced NMR Spectroscopy as a Tool to Probe Silica Surface Heterogeneity (IC07)

15.15 **Jan Breitenfeld**, X. Hu, EPF Lausanne
Mechanistic Studies related to Nickel-Catalyzed Alkyl-Alkyl Cross Coupling Reactions (IC08)

15.30 **Katsiaryna Tarasava**, E. Freisinger, University of Zürich
Non-native Analogs of a Wheat Metallothionein (IC09)

15.45 **Amos Rosenthal**, H. Grützmacher, ETH Zürich
Indenyl Ruthenium and Nickel Complexes Bearing an Olefin Sidearm as a Steering Ligand (IC10)

16.00 **Shoubhik Das**, P. J. Dyson, G. Laurenczy, EPF Lausanne
Photochemical Reduction of CO₂: Facts and Future (IC11)

16.15 **Martino Rimoldi**, D. Fodor, J. van Bokhoven, A. Mezzetti, ETH Zürich
An Iridium (III) Hydride Pincer Complex Grafted on Mesoporous Silica as Single-Site Catalyst for Gas-Phase Olefin Hydrogenation (IC12)

16.30 **René M. Oetterli**, R. Alberto, F. Zelder, University of Zürich
Impact of structural modifications of Vitamin B12 on its physico-chemical properties and the biological activity (IC13)

16.45 **Michael Benz**, H. Braband, R. Alberto, University of Zürich
A novel synthetic pathway for the formation of water stable ⁹⁹Tc-NHC Complexes (IC14)

Medicinal Chemistry & Chemical Biology

Session Endowment: Actelion

11.00–13.00 **Session I (CE 6)**
Chair: **Karl-Heinz Altmann** (ETH Zürich)
Abstracts MC001–MC007

- 11.00–11.30** **Lecture of the KGF Senior Industrial Investigator Award Laureate 2013**
Ian Lewis
Novartis Institutes for Biomedical Research, Basel
SOM230: A new therapeutic modality for Cushing's disease
Abstract MC001
- 11.30** L. Pollaro, A. Angelini, K. Moala, **Christian Heinis**, EPF Lausanne
Directed evolution of bicyclic peptides for therapeutic application (MC002)
- 11.45** **Christian Lerner**, C. Bissantz, B. Büttelmann, F. Diederich, A. Gast, R. Jakob-Roetne, D. Roth, M. Rudolph, D. Schlatter, F. Hoffmann-La Roche, Basel and ETH Zürich
Non-nucleosidic COMT bisubstrate inhibitors (MC003)
- 12.00** **Thomas Jack**, M.-D. Ruepp, O. Mühlemann, A. J. Thomson, S. C. R. Lummis, M. Lochner, University of Bern and University of Cambridge
Synthesis and testing of photoaffinity probes for the site-selective chemical modifications of the 5-HT₃ receptor (MC004)
- 12.15** **Jean Quancard**, B. Bollbuck, D. Angst, P. Janser, F. Berst, P. Buehlmayr, M. Streiff, C. Beerli, V. Brinkmann, D. Guerini, P. A. Smith, T. Seabrook, M. Traebert, K. Seuwen, R. Hersperger, C. Bruns, F. Bassilana, M. Bigaud, Novartis Institutes for Biomedical Research, Basel
Discovery of Highly Potent SIP1 Receptor Antagonists With In Vivo Efficacy (MC005)
- 12.30** **Roland C. Preston**, F. P. C. Binder, M. Zierke, R. Jakob, T. Maier, B. Ernst, University of Basel
Structural Insights into E-selectin-Ligand Interactions (MC006)
- 12.45** **Guido Galley**, A. Goergler, M. C. Hoener, R. D. Norcross, H. Stalder, F. Hoffmann-La Roche, Basel
Imidazolines and Imidazoles as TAAR1 Agonists (MC007)
- 13.00–14.30** **Poster session (CE SPO)**
Abstracts MC016–MC100
- 15.00–17.00** **Session II (CE 6)**
Chair: **Yves Auberson** (Novartis Institutes for Biomedical Research)
Abstracts MC008–MC016
- 15.00** P. Risch, H. Fretz, T. Pfeifer, **Julien Pothier**, Actelion Pharmaceuticals Ltd., Allschwil
Structure elucidation of two major metabolites of CRTh2 antagonist ACT-129968 (Setipiprant) (MC009)
- 15.15** **Solène Passemard**, D. Staedler, G. Sonogo, J. Loup, L. Juillerat-Jeanneret, S. Gerber-
Lemaire, EPF Lausanne and University Hospital Lausanne
Functionalized nanomaterials for cancer diagnosis (MC008)
- 15.30** **Raphael M. Franzini**, W. Decurtins, M. Wichert, F. Samain, J. Scheuermann, D. Neri, ETH Zürich and Philochem AG, Otelfingen
Development and Evaluation of DNA-Encoded Compound Libraries as an Effective Drug-Discovery Method (MC010)
- 15.45** **Olivier Simić**, T. Brandl, P. Rigollier, U. Bodendorf, N. Schiering, C. Ehrhardt, U. Hassiepen, K. Lin, J. Flynn, Novartis Institutes for Biomedical Research, Basel
Identification of novel P3-P1' macrocyclic inhibitors of HCV NS3/4A protease (MC011)
- 16.00** **Gražvydas Lukinavičius**, K. Umezawa, L. Reymond, K. Johnsson, EPF Lausanne
Applications of silicon-rhodamine for the imaging of living cells (MC012)
- 16.15** W. Haap, G. Hartmann, R. Alvarez Sanchez, L. Anselm, D. W. Banner, R. Ecabert, U. Grether, H. Kuehne, B. Kuhn, **Thomas Luebbbers**, J. U. Peters, J. M. Plancher, A. Rufer, B. Spinnler, F. Hoffmann-La Roche AG, Basel
Discovery of highly potent and selective covalent reversible cathepsin S inhibitors (MC013)
- 16.30** **Sébastien Tardy**, W. H. Bisson, L. Mologni, P. Goekjian, C. Gambacorti-Passerini, L. Scapozza, University of Geneva, University of Milan-Bicocca and University of Lyon
Synthesis of inhibitors of oncogenic fusion protein NPM-ALK for in vitro and in vivo assays (MC014)
- 16.45** L. C. Bouchez, **Marion Rusch**, M. Pastor, M. Livendahl, C. Bodenreider, D. Hoepfner, Novartis Institutes for Biomedical Research
Total Synthesis of the Antimalarial Agent Cladosporin (MC015)
- 17.00** **Martin G. Nussbaumer**, A. Mascarin, T. Mindt, N. Bruns, University of Basel
Thermosome – a cage protein acting as a versatile delivery platform (MC016)

Organic Chemistry
Session A: Catalytic methodologies and sustainable processes

Session Endowment: INEOS

11.00–13.00 **Session I (CE 5)**
Chair: **Jieping Zhu** (EPF Lausanne)
Abstracts OC004–OC011

11.00 **Axelle Cotte**, D. Jeannerat, University of Geneva

- A new approach to separate chemical shift and scalar coupling of 1D proton NMR spectra* (OC004)
- 11.15** T. A. Schaub, F. Hampel, **Milan Kivala**, University of Erlangen-Nürnberg
Phosphorus-doped π -conjugated organic architectures (OC005)
- 11.30** **Rémi Vanel**, F.-A. Miannay, E. Vauthey, J. Lacour, University of Geneva
Synthesis and properties of novel indol-triarylcarbenium ions (OC006)
- 11.45** **Yingjie Zhao**, Y. Domoto, E. Orentas, N. Sakai, S. Matile, University of Geneva
Catalysis with Anion- π Interactions (OC007)
- 12.00** **Baihua Ye**, N. Cramer, EPF Lausanne
Chiral Cp-ligands: stepping stone for asymmetric Rh(III)-catalyzed C-H functionalization (OC008)
- 12.15** **Antoine Derible**, J.-M. Becht, C. Le Drian, University of Haute-Alsace, Mulhouse
Magnetically recoverable, reusable, Pd catalysts for Suzuki couplings (OC009)
- 12.30** K. Tishinov, N. Fei, S. Geigle, **Dennis Gillingham**, University of Basel
Catalytic Alkylation of Nucleic Acids (OC010)
- 12.45** **David Grassi**, A. Alexakis, University of Geneva
Transition metal-free Asymmetric Allylic Alkylation using Grignard reagents. What you cannot do using conventional metal catalyzed process (OC011)
- 13.00–14.30** **Poster session (CE SPO)**
Abstracts OC031–OC104
- 15.00–17.00** **Session II (CE 5)**
Chair: **Greet Van Eetvelde** (INEOS)
Abstracts OC001, OC012–OC017
- 15.00–15.30** *Invited Lecture*
John McNally
INEOS, Rolle
INEOS Technologies: provider of sustainable polyolefin technology solutions
Abstract OC001
- 15.30** **Houhua Li**, C. Mazet, University of Geneva
Iridium-catalyzed Double Diastereoselective Isomerization of Primary Allylic Alcohols (OC012)
- 15.45** **Bo Yao**, Q. Wang, J. Zhu, EPF Lausanne
Palladium-Catalyzed Coupling of ortho-Alkynylanilines with Terminal Alkynes Under Aerobic Conditions: Efficient Synthesis of 2,3-Disubstituted 3-Alkynyloindoles (OC013)
- 16.00** **Lijun Zhou**, Y. Zou, Q. Wang, A. Goeke, Fudan University and Givaudan Flavors (Shanghai)

Iron(III) Chloride Catalyzed Oxonia-Prins Cyclization Reaction (OC014)

- 16.15** **Robert Kastl**, H. Wennemers, ETH Zürich
Peptide-catalyzed Stereoselective Conjugate Addition Reactions Generating All-Carbon Quaternary Stereogenic Centers (OC015)
- 16.30** **Hailing Li**, A. Alexakis, University of Geneva
Copper-Catalyzed Enantioselective Synthesis of Axially Chiral Allenes (OC016)
- 16.45** **Cecilia Tortoreto**, T. Achard, A. Poblador-Bahamonde, L. Guénée, J. Lacour, University of Geneva
Unexpected 3-Atoms Insertion of Ru-Metal Carbenes into Epoxides (OC017)

Organic Chemistry Session B: Synthetic methodologies and applications

Session Endowment: SYNGENTA

- 11.00–13.00** **Session I (CE 106)**
Chair: **Christian Bochet** (University of Fribourg)
Abstracts OC002, OC018–OC024
- 11.00–11.15** *Lecture of the KGF Industrial Investigator Award Laureate 2013*
Mark Rogers-Evans
F. Hoffmann-La Roche, Basel
The Concept and Use of Compact Modules at Roche
Abstract OC002
- 11.15** **Zbigniew Pianowski**, B. Wörsdörfer, D. Hilvert, ETH Zürich
Efficient in Vitro Encapsulation of Protein Cargo by an Engineered Protein Container (OC018)
- 11.30** **Samad Ebrahimi**, M. M. Farimani, F. Mirzania, M. Hamburger, University of Basel and Shahid Beheshti University, Tehran
*New sesterterpenoids from *Salvia mirzayanii* - stereochemical characterization by computational electronic circular dichroism* (OC019)
- 11.45** **Gabriel Schäfer**, C. Matthey, J. W. Bode, ETH Zürich
The Addition of Grignard Reagents to Isocyanates (OC020)
- 12.00** **Gregor Kiefer**, L. Jeanbouquin, K. Severin, EPF Lausanne
Oxidative Coupling Reactions of Grignard Reagents with Nitrous Oxide (OC021)
- 12.15** **Wangqing Kong**, P. Feige, T. de Haro, C. Nevado, University of Zürich
Regio-, Enantioselective Aminofluorination of Alkenes (OC022)

- 12.30** **Elia Janett**, C. G. Bochet, University of Fribourg
Towards a DNA-Based Bacterial Sensor (OC023)
- 12.45** **Hideki Miyatake-Ondo**zabal, L. M. Bannwart, K. Gademann, University of Basel
Enantioselective Total Synthesis of Virosaine A and Related Natural Products (OC024)
- 13.00–14.30** **Poster session (CE SPO)**
Abstracts OC031–OC104
- 15.00–17.00** **Session II (CE 106)**
Chair: **Damien Jeannerat** (University of Geneva)
Abstracts OC003, OC025–OC030
- 15.00–15.30** **Invited lecture**
Clemens Lamberth
Syngenta Crop Protection AG, Stein
Mono- and biheterocyclic tubulin polymerization promoters: design aspects, synthesis and fungicidal activity
Abstract OC003
- 15.30** **Gong Xu**, M. Lüthy, J. Habegger, P. Renaud, University of Bern
Generation of 1-Chloroalkyl Radicals from Organoboranes (OC025)
- 15.45** **Caroline Souris**, F. Frébault, D. Audisio, N. Maulide, Max-Planck-Institut für Kohlenforschung, Mülheim
Stereodefined Synthesis of Functionalized Dienes: Streamlining Access to Polyene Natural Products (OC026)
- 16.00** **Florian de Nanteuil**, J. Waser, EPF Lausanne
Synthesis and Reactivity of Nitrogen-Substituted Small Rings (OC027)
- 16.15** **Václav Matoušek**, E. Pietrasiak, J. Charpentier, R. Schwenk, A. Togni, ETH Zürich
Optimized Synthesis of Hypervalent Iodine Reagents for Electrophilic Trifluoromethylation (OC028)
- 16.30** **Raphael Schiess**, K.-H. Altmann, ETH Zürich
Towards the Total Synthesis of New Cembranolides (OC029)
- 16.45** **Lukas Felix**, M. Arndt, M. Mayor, University of Basel and University of Vienna
Multi-Porphyrin Systems for Matter-Wave Interferometry (OC030)
- 11.00** **P. Morten Hundt**, M. E. Van Reijzen, R. D. Beck, EPF Lausanne
Vibrationally Promoted Chemisorption of Water on Ni(111) (PC01)
- 11.15** A. Kushnarenko, E. Miloglyadov, M. Quack, **Georg Seyfang**, ETH Zürich
Intramolecular Vibrational Redistribution in Polyatomic Molecules Measured in Femtosecond Pump-Probe Experiments (PC02)
- 11.30** **Pierre-André Cazade**, M. Meuwly, University of Basel
Computational 2D-IR Spectroscopy of NMA in Solution (PC03)
- 11.45** **Philipp Kowalewski**, H.-M. Frey, S. Leutwyler, University of Bern
Accurate Structure of n-Hexane by Femtosecond Rotational Raman Spectroscopy (PC04)
- 12.00** **Oleg Aseev**, T. Rizzo, EPF Lausanne
Using Cold-Ion Spectroscopy to Unravel the Mechanism of Peptide Sequence Scrabbling in Collision Induced Dissociation (PC05)
- 12.15** **Clément Lauzin**, B. Gans, F. Merkt, ETH Zürich
PFI-ZEKE Photoelectron Spectra of H₂O⁺ in the First Excited Electronic State (\tilde{A}^2A_1) (PC06)
- 12.30** **Benjamin Bertsche**, A. Osterwalder, EPF Lausanne
Merged-Beam Experiments of Neutral Particles (PC07)
- 12.45** **Short talks**
- Johannes Seibel** (PC08)
Noelia Barrabes (PC09)
Ana Gamiz Hernandez (PC10)
Radmila Janečková (PC11)
Thomas Nauser (PC12)
- 13.00–14.30** **Poster session (CE 101)**
Abstracts PC08–PC12, PC21–PC74
- 15.00–17.00** **Session II (CE 4)**
Chair: **Jacques-Edouard Moser** (EPF Lausanne)
Abstracts PC13–PC20
- 15.00** **Sami Jannin**, A. Bornet, J. Milani, R. Melzi, A. J. Perez Linde, P. Hautle, B. Van den Brandt, G. Bodenhausen, EPF Lausanne, Bruker Italia, PSI Villigen and Ecole Normale Supérieure, Paris
Dissolution Dynamic Nuclear Polarization off the Beaten Tracks (PC13)
- 15.15** **Tomáš Šolomek**, C. G. Bochet, T. Bally, University of Fribourg
Photochemistry of o-Nitrobenzyl Photoremovable Protecting Groups (PC14)

Physical Chemistry

- 11.00–13.00** **Session I (CE 4)**
Chair: **Frédéric Merkt** (ETH Zürich)
Abstracts PC01–PC12

- 15.30** **Romain Letrun**, E. Vauthey, University of Geneva
Anti-Kasha Behaviour in Photoinduced Bimolecular Electron Transfer Reactions (PC15)
- 15.45** **Christopher Arrell**, J. Ojeda, W. Okell, T. Witting, T. Siegel, Z. Diveki, R. Chapman, S. Hutchinson, F. Van Mourik, C. Cacho, E. Turcu, E. Springate, J. W. G. Tisch, J. P. Marangos, M. Chergui, EPF Lausanne, Imperial College London and STFC Rutherford Appleton Laboratory
Femtosecond H-Bond Dynamics in Liquid Water (PC16)
- 16.00** **Margherita Oraziotti**, A. Rodenberg, M. Guttentag, C. Bachmann, R. Alberto, P. Hamm, University of Zürich
Investigating the Mechanism of Hydrogen Evolution of Cobalt Based Catalysts (PC17)
- 16.15** **Nam Hee Kwon**, H. Yin, K. M. Fromm, University of Fribourg
Nano-LiMnPO₄ and Graphene Composite as Alternative Cathode Material for Lithium Ion Batteries (PC18)
- 16.30** **Susan Blaser**, H.-M. Frey, S. Leutwyler, University of Bern
Fluorescence Lifetime Measurement of Nucleobase Analogues using a Picosecond Streak Camera (PC19)
- 16.45** **Ahmad Ajdarzadeh**, A. Paraecattil, J. C. Brauer, J.-E. Moser, EPF Lausanne
Time-Resolved THz Studies of Electron Transfer Dynamics at Dye-Sensitized TiO₂ Nanoparticle Surfaces: Evidence for the Formation and Dissociation of Interfacial Charge Transfer Excitons (PC20)
- 11.55** **Mohsen Moazzami Gudarzi**, F. J. M. Ruiz-Cabello, P. Maroni, M. Borkovec, University of Geneva
Failure of DLVO Theory at Distance of Few Nanometers: a Colloidal Probe Study (PCI04)
- 12.10** **Marco Furlan**, M. Lattuada, University of Fribourg
Nacre-Like Composite Materials Produced via Magnetically-Controlled Phase Separation of Sol-Gel Process (PCI05)
- 12.25** **Thomas Schuster**, S. Sigg, W. Meier, University of Basel
Purely Peptidic Amphiphiles: from Self-Assembled Structures to Gene Delivery (PCI06)
- 12.40** **Ana Maria Raduta**, S. Hanke, K. M. Arndt, H.-H. Klok, EPF Lausanne and University Potsdam
Polymer-Mediated Delivery of Therapeutic Coiled Coils (PCI07)
- 13.00–14.30** **Poster session (BS 170)**
Abstracts PCI13–PCI65
- 15.00–17.00** **Session II (BS 160)**
Chair: **Holger Frauenrath** (EPF Lausanne)
Abstracts PCI02, PCI08–PCI12
- 15.00–15.40** **Invited lecture**
Annette Schmidt
University of Cologne, Germany
Motion and Balance of Complex Fluids on the Nanoscale
Abstract PCI02
- 15.40** **Stephen Schrettl**, H. Frauenrath, EPF Lausanne
Low-Temperature Preparation of Carbon Nanosheets from Hexa(ethynylene) Amphiphiles (PCI08)
- 15.55** **Zhikun Zheng**, A. Rossi, J. Sakamoto, A. D. Schlüter, ETH Zürich
Synthesis of Monolayer Metal-Organic Polymer/Copolymer Sheets (PCI09)
- 16.10** **Andrea Gasperini**, K. Sivula, EPF Lausanne
Controlling the Microstructure and Charge Carrier Transport of Solution-Processed Semiconducting Polymers (PCI10)
- 16.25** **Dorina M. Opris**, S. Dünki, F. Nüesch, J. E. Q. Quinsaat, Y. Song Ko, S. Michel, C. Racles, M. Cazacu, EMPA Dübendorf and Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
Dielectric Elastomers Put to Work (PCI11)
- 16.40** **Alexandru Zabara**, R. Negrini, O. Onaca-Fischer, R. Mezzenga, ETH Zürich and University of Basel
Perforated Bicontinuous Cubic Phases with pH-Responsive Topological Channel Interconnectivity (PCI12)

Polymers, Colloids & Interfaces

Session Endowment: Dow

- 11.15–13.00** **Session I (BS 160)**
Chair: **Frank Scheffold** (University of Fribourg)
Abstracts PCI01, PCI03–PCI07
- 11.00–11.40** **Invited lecture**
Günter K. Auernhammer
Max Planck Institute for Polymer Research, Mainz, Germany
Single Particle Tracking in Colloidal and Granular Matter under External Load
Abstract PCI01
- 11.40** **Philipp Anstaett**, Y. Zheng, T. Thai, A. M. Funtson, U. Bach, G. Gasser, University of Zürich and Monash University, Clayton
Peptide Nucleic Acid Modified Gold Nanoparticles and their Assembly on Surfaces (PCI03)