SCS FALL MEETING 2016 CHIMIA 2016, 70, No. 7/8 527

11.15

## Award Lectures Overview

09.55 SCS Honorary Member 2016
Prof. E. Peter Kündig,
University of Geneva
«Whole New Landscapes»
Plenary Session [PS-001],
lecture hall G30.



The honorary membership is given in recognition of Prof. E. Peter Kündig's research achievements in organic synthesis and catalysis with transition metals and to honor his far-ranging and thoughtful management as president of the Platform Chemistry of the Academy of Natural Sciences in the years 2007–2009 and as president of the Swiss Chemical Society in the past 6 years since 2010.

10.30 Sandmeyer Award Lecture 2016
Dr. Martin Weibel, Dr. Robert Flatt, Dr. Hendrik
Heinz, Sika Technology AG
«Development of new commercial organic additives for the grinding of inorganic solids»
Plenary Session [PS-002], lecture hall G30.
The award is given to the team comprising researchers from Sika Technology AG, ETH Zurich and the University of Colorado Boulder for their experimental and modeling studies of new commercial organic additives for the grinding of inorganic solids.

11.15 KGF-SCS Senior Industrial Science Award Lecture 2016 Dr. Eric Francotte, Novartis Pharma AG «Chromatographic resolution

> of racemic compounds on optically active polymers as chiral



stationary phases»
Session of Analytical Sciences, [AS-011], lecture hall G95.

The award is given for Dr. Francotte's outstanding contributions to chromatographic resolution of racemic compounds on optically active polymers as chiral stationary phases and his pioneering work in implementing new preparative chromatographic techniques.

11.15 KGF-SCS Senior Industrial Science Award Lecture 2016 Prof. Peter Nesvadba, BASF Schweiz AG «Radicals in the Life of Industrial Polymer»,



Session of Polymers, Colloids & Interfaces, [PI-011], lecture hall G55.

The award is given for Prof. Nesvadba's groundbreaking contributions to the discovery and development of novel stabilizers for monomers and polymers, novel dyes, first industrial realization of controlled radical polymerization, to the development of safe alternatives to organic peroxides and for his engagement as bridge builder between academia and industry.

KGF-SCS Industrial Science Award Lecture 2016 Dr. Martin H. Bolli, Actelion Pharmaceuticals Ltd «The Discovery of Macitentan - A Standard Medicinal Chemistry Approach?»



Session of Medicinal Chemistry & Chemical Biology [MC-012], lecture hall G60.

The award is given for Dr. Bolli's excellent contributions in medicinal chemistry culminating in the discovery and development of Macitentan, a drug for the treatment of pulmonary arterial hypertension.

11.15 KGF-SCS Industrial Science Award Lecture 2016 Dr. Andreas Herrmann, Firmenich SA «Profragrance chemistry as interdisciplinary research area and key technology for



**fragrance delivery**», Session of Organic Chemistry, [OC-011], lecture hall G45.

The award is given for Dr. Herrmann's essential contributions to make profragrance chemistry an interdisciplinary research area and to establish it as a key technology for fragrance delivery.

17.00 Paracelsus Award Lecture 2016
Prof. Michael Graetzel, EPF
Lausanne
«Invention and development of
the dye-sensitized solar cells»,
Plenary Lecture, lecture hall G30.

The award is given for Prof. Graet-



zel's invention and development of the dye-sensitized solar cell.

Plenary Sessions – G30 Chair: Dr. Hans Peter Lüthi, Prof. Roger Alberto



Session Endowment: Givaudan Suisse SA

09.55 «Whole New Landscapes» (Lecture of the SCS Honorary Member 2016) [PS-001]
Prof. E. Peter Kündig, University of Geneva

10.30 Sandmeyer Award Lecture 2016: «Development of new commercial organic additives for the grinding of inorganic solids» [PS-002]
Dr. Martin Weibel, Dr. Robert Flatt, Dr. Hendrik Heinz, Sika Technology AG

17.00 Paracelsus Award Lecture 2016: «Invention and development of the dye-sensitized solar cells» [PS-003]
Prof. Michael Graetzel, EPF Lausanne

## **Abstract codes**

PS

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

Plenary Session

528 CHIMIA 2016, 70, No. 7/8 SCS FALL MEETING 2016

# PARALLEL SESSIONS

#### **Analytical Sciences [AS]**

**Morning Session - G95** 

Chair: Dr. Hanspeter Andres

No Session Endowment

11.15 Chromatographic resolution of racemic compounds on optically active polymers as chiral stationary phases [AS-011]
Eric Francotte, Novartis Institutes for Biomedical Research

11.45 Towards a better understanding of spectral similarity between structurally related compounds [AS-013]
Jennifer E. Schollée, Eawag, Dübendorf (J. Hollender)

12.00 Understanding the cellular distribution and protein targets of a ruthenium (II) anti-cancer compound, RAPTA-T via mass spectrometry [AS-014]
Ronald F. S. Lee, EPF Lausanne (P. J. Dyson)

12.15 Combined GC- and UHPLC-HR-MS based metabolomics to analyze durable anti-fungal resistance processes in cereals [AS-015]
Rahel Bucher, University of Zurich (B. Keller)

12.30 Compound-specific isotope analysis of environmental organic micropollutants: challenges and possibilities [AS-016]
Rani Bakkour, Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf (T. Hofstetter)

# Afternoon Session - G95

Chair: Dr. Stefan Schürch

15.15 Electrochemical Proton Transfer Based Polyaniline Films for Thin Layer Titrations [AS-022] Majid Ghahraman Afshar, University of Geneva (E. Bakker)

15.30 Persistent organic pollutants in white-blooded Antarctic fish Champsocephalus gunnari and Chaenocephalus aceratus [AS-023]

Markus Zennegg, Empa

15.45 Field-scale *in situ* analysis of ambient N2O isotopic composition to trace source processes in an intensively managed grassland [AS-024]
Erkan Ibraim, Empa (J. Mohn)

16.00 At the interface between climate research and metrology: Gas adsorption and desorption on high pressure standard cylinders [AS-025] Ece Satar, University of Bern Physics Institute (H. Andres)

16.15 Enyzme-Substrate Complexes Studied by Native Electrospray Mass Spectrometry: First Steps
Towards Gas-Phase Enzymology [AS-026]
Martin Francis Czar, ETH Zurich (R. Zenobi)

16.30 Studies on discrete samples using a microdroplet generator combined with ICP-Time-of-Flight Mass Spectrometry [AS-027]
Lyndsey Hendriks, ETH Zurich (D. Günther)

#### **Computational Chemistry [CC]**

# **Morning Session - G91**

Chair: Dr. Ivano Tavernelli



Session Endowment: Materials Design

11.15 Industrial Impact of Computational Chemistry and Materials Science [CC-011]
Erich Wimmer, Materials Design s.a.r.l.

11.45 **Balancing London dispersion and the delocali- zation error with DFT functionals [CC-013]**Alberto Fabrizio, EPF Lausanne (*C. Corminboeuf*)

12.00 A fast scheme for approximated Fock exchange potentials in plane wave implementations of Kohn-Sham Density Functional Theory [CC-014] Martin Bircher, EPF Lausanne (U. Röthlisberger)

12.15 Quantitative Reaction Energies from an Automated Multi-Configurational Approach [CC-015]
Christopher Stein, ETH Zurich (M. Reiher)

12.30 **FDE-ADC:** Multiscale density embedding with an accurate wavefunction method. [CC-016] Alexander Zech, University of Geneva (T. A. Wesolowski)

#### Afternoon Session - G91

Chair: Dr. Marcella Iannuzzi

15.00 Industrial modeling aspects of 1,3-dicarbonyl compounds [CC-021]
Christoph Taeschler, Lonza AG

15.30 Is oxide hydrogenation equivalent to reduction?
Fundamental differences between TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub>
from DFT [CC-023]
Clelia Spreafico, ETH Zurich (*J. VandeVondele*)

15.45 Interatomic many-body representation improves molecular machine learning models [CC-024]
Bing Huang, University of Basel (O. Lilienfeld)

16.00 Reactive Molecular Dynamics and Infrared Spectra of Double Proton Transfers with Coupling Effects [CC-025]
Zhen-Hao Xu, University of Basel (M. Meuwly)

16.15 On the ultrashort pulse approximation for the interaction of molecule with pulsed laser fields: Generalization of the Franck-Condon principle [CC-026]

Aurélien Patoz, EPF Lausanne (J. Vanicek)

16.30 Dry Reforming and Competitive Reactions on Ni, Pd and Pt metal Surfaces from DFT Calculations and Microkinetic Modeling Simulations [CC-027]

Aleix Comas-Vives, ETH Zurich

SCS FALL MEETING 2016 529 CHIMIA 2016, 70, No. 7/8

# Catalysis Sciences & **Engineering [CE]** Morning Session - G20

# **CLARIANT**

Chair: Prof. Christoph Müller

Session Endowment: Clariant International Ltd.

In situ Studies on the Behavior of Metal/Oxide 11.15 Catalysts during the Water-gas Shift Reaction [CE-011] José A. Rodriguez, Brookhaven National Laboratory, **USA** 

Parahydrogen-based hypersensitive NMR/MRI 11.45 toolkit for catalysis [CE-013] Igor V. Koptyug, International Tomography Center, Novosibirsk, Russia

12.15 A closure to the controversy around hydrogen spillover: a nanolithography and single nanoparticle spectro-microscopy approach [CE-015] Waiz Karim, ETH Zurich/PSI Villigen (J. A. van Bokhoven)

12.30 Photoelectrochemical Water Splitting from Earth-Abundant CuO Thin Film Photocathode: **Enhancing Performance and Photo-stability** through Deposition of Overlayers [CE-016] Wilman Septina, University of Zurich (D. Tiley)

12.45 Why Size Matters and Favors CO Activation on Larger Ru Nanoparticles: A Molecular Understanding from First Principles [CE-017] Lucas Foppa, ETH Zurich (C. Copéret)

# Afternoon Session - G20

Chair: Dr. Alexey Fedorov

15.00 Modelling the Phosphorous Dynamics of Vanadyl Pyrophosphate Catalysts [CE-021] Gerhard Mestl, Clariant Produkte (Deutschland) **GmbH** 

15.30 On purpose CO production via methane oxychlorination over heterogeneous catalysts [CE-023] Vladimir Paunovic, ETH Zurich (J. Pérez-Ramírez)

15.45 Rational design of ceria-based supported noble metal catalysts for low temperature CO oxidation using transient X-ray absorption spectroscopy [CE-024] René Kopelent, Paul Scherrer Institute, Villigen (O. V. Safonova)

TiO, nanocontainers and nanospheres as photocat-16.00 alysts for CO, reduction and photoelectrochemical water splitting: Structural modification [CE-025] Nelly Hérault, University of Fribourg (K. M. Fromm)

16.15 Understanding of the role of Fe in highly active and stable Ni-Fe dry reforming catalysts [CE-026] Sung Min Kim, ETH Zurich (C. Müller)

16.30 Chemical layer deposition of porous alumina overcoats increases activity and stability in liquid phase catalytic conversion of biomass-derived chemicals [CE-027] Florent Héroguel, EPF Lausanne (J. Luterbacher)

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

No Session Endowment

11.15 Natural Born Catalysts: Photocatalytic Water Oxidation by Molecular Metal Oxides [IC-011] Marcella Bonchio, University of Padova, Italy **High Oxidation State N-Heterocyclic Carbene** 11.45

Molybdenum Alkylidene Complexes: Functional **Group-Tolerant Olefin Metathesis Catalysts** [IC-013] Suman Sen, University of Stuttgart

12.00 Silver(I) N-heterocyclic complexes for C-C bond activation of alkylnitriles and catalytic application in oxazoline synthesis [IC-014] Rachael Heath, University of Bern (M. Albrecht)

12.15 **C-H Activations Catalyzed by Transition-Metal Ions Isolated on Metal Oxide Surfaces [IC-015]** Deven Paul Estes, ETH Zurich

12.30 Exploring Trifluoromethylthioethers as ligands -Platinum(II) complexes of 8-(trifluoromethylthio) quinoline [IC-016] Carl Philipp Rosenau, ETH Zurich (A. Togni)

#### Afternoon Session - G30

Chair: Prof. Bruno Therrien

15.00 **D-Glucose-Platinum(II) Conjugates for Targeted Delivery of Platinum to Cancer Cells [IC-021]** Malay Patra, Massachusetts Institute of Technology / University of Zurich (S. J. Lippard)

Red-light activated photoCORMs of Mn(1) species 15.15 bearing symmetric substituted 2,2'-azopyridines [IC-022] Emmanuel Kottelat, University of Fribourg (F. Zobi)

15.30 Not so similar after all. Fundamental differences in reactivity of fac-[M(solvent)<sub>3</sub>(CO)<sub>3</sub>]+  $(M = Re, {}^{99}Tc)$  with CO [IC-023] Angelo Frei, University of Zurich (R. Alberto)

15.45 Controlling architecture of coordination cages via the aspect ratio of the ligands [IC-024] Suzanne Maria Jansze, EPF Lausanne (K. Severin)

16.00 **Design Approaches to Blue and White Light Emitting Gold(III) Complexes [IC-025]** Michael Bachmann, University of Zurich (K. Venkatesan)

16.15 Anthracene-based ligands for new luminescent coordination polymers [IC-026] Serhii Vasylevskyi, University of Fribourg (K. Fromm)

Beyond size effects: composition-tunable 16.30 properties for quaternary Cu-Zn-In-Se quantum dots [IC-027] Maksym Yarema, ETH Zurich (V. Wood)

SCS FALL MEETING 2016 530 CHIMIA 2016, 70, No. 7/8

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



Session Endowment: Actelion Ltd

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

#### Afternoon Session - G60

Chair: Prof. Jean-Louis Reymond

- 15.00 **Optimization of 1,4-Disubstituted Benzodiazepines** as Selective and Brain Penetrant Triple Calcium T-Channel Blockers [MC-021] Romain Siegrist, Actelion Pharmaceuticals Ltd.
- A FUC/LecB system to crystallize versatile nucleic 15.15 acid structures [MC-022]

Pascal Röthlisberger, Institut Pasteur (M. Hollenstein)

Synthesis and oomycete fungicidal activity of 15.30 a new family of inhibitors targeting an oxysterol binding protein [MC-023]

Martin Pouliot, Syngenta Crop Protection

Stereoselective Synthesis and Biological Evaluation 15.45 of Highly Potent New (-)-Zampanolide Derivatives [MC-024]

Tobias Brütsch, ETH Zurich (K.-H. Altmann)

16.00 High Kinetic Stability of T-HgII-T and DNA **Polymerase Inhibition [MC-025]** Olivia Paula Schmidt, University of Zurich

(N. W. Luedtke)

16.15 Discovery of a Potent and Selective Reversible **BTK Inhibitor for the Treatment of Autoimmune** Diseases [MC-026]

Robert Pulz, Novartis Institutes for Biomedical Research

16.30 **Investigations for New Therapeutic Targets** for Neurodegenerative Disease. [MC-027] Erika Crane, University of Basel (K. Gademann)

# Organic Chemistry [OC]

Morning Session - G45 Chair: Prof. Cristina Nevado



Session Endowment: Syngenta Crop Protection AG

Profragrance chemistry as interdisciplinary 11.15 research area and key technology for fragrance delivery [OC-011]

Andreas Herrmann, Firmenich SA

Helically Chiral Open-Shell Polycyclic Aromatic 11.45 **Hydrocarbons [OC-013]** 

Prince Ravat, University of Basel

- 12.00 **Chiral Ruthenium-cyclopentadienyl Complexes** as Versatile Catalysts for Enantioselective Transformations [OC-014] David Kossler, EPF Lausanne
- 12.15 **Inverse Electron-Demand [4 + 2]-Cycloadditions** of Ynamides: Access to Novel Pyridine Scaffolds [OC-015] Guillaume Duret, Strasbourg University (N. Blanchard)
- 12.30 Stereoselective Arene-Forming Aldol Condensation: Synthesis of Configurationally Stable Oligo-1,2-naphthylenes [OC-016] Dominik Lotter, University of Basel (C. Sparr)

# Afternoon Session - G45

Chair: Prof. Olivier Baudoin

15.00 **Optimization of Manganese Coupling Reaction for** Kilogram-scale Preparation of two Aryl-1,3-dione **Building Blocks [OC-021]** 

Tomas Smejkal, Syngenta Crop Protection AG

15.30 **Mechanosensitive Fluorescent Membrane Probes** [OC-023]

Quentin Verolet, University of Geneva (S. Matile)

Metal-Catalyzed Stereoselective Dicarbofunction-15.45 alization of Alkynes [OC-024]

Andrés García-Domínguez, University of Zurich

Development and applications of C(sp<sup>3</sup>)-H 16.00 Alkenylation [OC-025]

David Dailler, University of Basel (O. Baudoin)

16.15 A family of low molecular-weight, organic catalysts for reductive C-C and C-N bond formation [OC-026]

Saad Shaaban, University of Vienna (N. Maulide)

16.30 Size-controlled nanoparticle formation in aqueous media with a thiol-free tripeptide [OC-027] Stefano Corrà, ETH Zurich

SCS FALL MEETING 2016 CHIMIA 2016, 70, No. 7/8 531

## **Physical Chemistry [PC]**

Morning Session - G40

Chair: Prof. Samuel Leutwyler



Session Endowment: Bruker BioSpin

- 11.15 Time-resolved X-ray absorption spectroscopy indicates a new photodissociation mechanism of dissolved CBr<sub>4</sub> [PC-011]
  Rok Bohinc, Paul Scherrer Institute
  (J. A. van Bokhoven)
- 11.30 Reaction-detected infrared spectroscopy of state-selected molecular ions [PC-012]
  Ugo Jacovella, ETH Zurich (F. Merkt)
- 11.45 From non-relativistic pre-Born-Oppenheimer theory to molecular structure [PC-013]
  Andrea Muolo, ETH Zurich
- 12.00 Towards hybrid trapping of cold molecules and cold molecular ions [PC-014]
  Dominik Haas, University of Basel (S. Willitsch)
- 12.15 State-to-state scattering of methane from Ni(111) and epitaxial graphene on Ni(111) [PC-015]

  Maarten van Reijzen, EPF Lausanne (R. Beck)
- 12.30 Study of the N(<sup>4</sup>S)+NO(<sup>2</sup>II) reactive collision at extreme temperatures relevant to the hypersonic flight regime. [PC-016]
  Otoniel Denis-Alpizar, University of Basel (M. Meuwly)

# Afternoon Session - G40

Chair: Prof. Frédéric Merkt

- 15.00 Spectroscopic separation of <sup>13</sup>C NMR spectra of complex isomeric mixtures by the CSSF-TOCSY-INEPT experiment [PC-021]
  Aitor Moreno, Bruker BioSpin Corp
- 15.30 Ultrafast spectroscopy as a tool to investigate the microstructure of donor-acceptor blends for organic photovoltaics [PC-023]

  Martina Causa, University of Fribourg (N. Banerji)
- 15.45 Surface-Enhanced 2D Attenuated Total Reflectance IR Spectroscopy for Studying Surface-Sensitive Ultrafast Vibrational Dynamics [PC-024] Jan Philip Kraack, University Zurich
- 16.00 Direct visualization of excited-state symmetry breaking by ultrafast time-resolved infrared spectroscopy [PC-025]

  Bogdan Dereka, University of Geneva (E. Vauthey)
- 16.15 Rational Design of Nitroxide Biradicals for Efficient Cross-Effect Dynamic Nuclear Polarization [PC-026]

  Dominik Józef Kubicki, Ecole polytechnique fédérale de Lausanne (O. Ouari)
- 16.30 Microhydration of N1-Cytosine Derivatives [PC-027]
  Luca Siffert, University of Bern (S. Leutwyler)

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

Chair: Prof. Markus Niederberger



Session Endowment: Dow Europe GmbH

- 11.15 **Radicals in the Life of Industrial Polymer [PI-011]**Peter Nesvadba, BASF Schweiz AG
- 11.45 Selective attachment of Gold Nanoparticles on Asymmetrically Functionalized Janus Nanoparticles [PI-013] Florian Guignard, Adolphe Merkle Institute -

Florian Guignard, Adolphe Merkle Institute - University of Fribourg (M. Lattuada)

- 12.00 Multi-stimuli responsive films designed through layer-by-layer assembly of PAA-b-PNIPAM block copolymers for biomedical applications [PI-014]
  Alina Osypova, Empa
- 12.15 Developing New Strategies to study colloidal
  Nanocrystals using Dynamic Nuclear Polarization
  NMR Spectroscopy [PI-015]
  Laura Piveteau, ETH Zurich (C. Copéret)
- 12.30 Combined Electrical and Optical Characterization of Polydiacetylene [PI-016]
  Clément Girard-Reydet, Université de Genève (K. Sugihara)

#### Afternoon Session - G55

Chair: Prof. Andrei Honciuc

15.00 Retort tie-layer: the development of a solution for barrier retort structures [PI-021]

Eve Meric Kunsch, Dow Europe Grahl

Eva-Maria Kupsch, Dow Europe GmbH

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

Ralph Z Lange, ETH Zurich (A. D. Schlüter)