

PLENARY SESSIONS

Award Lectures

Lecture hall G30

Chairs: Prof. Christian Bochet

Dr. Alain De Mesmaeker

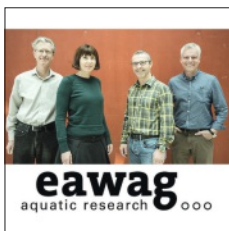
Sandmeyer Award Lecture 2019

Arsenic and other Geogenic Contaminants in Groundwater – a Global Challenge [PS-001]

September 6, 2019, 09.50–10.20h

Dr. Michael Berg, Dr. Stephan Hug, Dr. Annette Johnson (in memoriam), Dr. Andreas Voegelin and Prof. Lenny Winkel, from the Eawag, Dübendorf

The award is given for their experimental and modelling studies on drinking water contamination by arsenic and other geogenic elements with an enormous impact not only in Switzerland but around the globe.



SCS Industrial Science Award Lecture 2019

20 Years of Medicinal Chemistry – Always look at the bright side (of life) [PS-002]

September 6, 2019, 10.20–11.50h

Dr. Christoph Boss, Idorsia Pharmaceuticals Ltd.

The award is given to honor his outstanding contributions as medicinal chemists with remarkable analytical skills and an excellent flair for multidimensional lead optimization taking into consideration all aspects of modern medicinal chemistry.



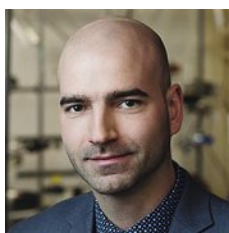
Grammaticakis-Neumann Award Lecture 2019

Photochemical Dearomatization of Nonactivated Arenes [PS-003]

September 6, 2019, 17.15–17.45h

Prof. David Sarlah, University of Illinois, Urbana, USA

Awarded for his great achievements in the development of photochemical dearomatization of nonactivated arenes that allows for a rapid incorporation of oxygen, nitrogen and carbon functionality with exquisite stereocontrol.



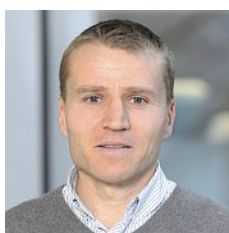
SCS Senior Industrial Science Award Lecture 2019

Alternative solvents: from a compliance-driven activity to a trigger for innovation [PS-004]

September 6, 2019, 17.45–18.15h

Dr. Fabrice Gallou, Novartis Pharmaceuticals AG, Basel,

Awarded in recognition of his outstanding track record of innovation and creativity in the field of organic synthesis and for his leadership in coaching and mentoring of young scientists at Novartis.



Abstract codes

AS	Analytical Sciences
CE	Catalysis Sciences & Engineering
CC	Computational & Theoretical Chemistry
IC	Inorganic Chemistry
MC	Medicinal Chemistry & Chemical Biology
OC	Organic Chemistry
PC	Physical Chemistry
PI	Polymers Colloids & Interfaces
[XY-011]...[XY-017]	Morning session lectures
[XY-021]...[XY-027]	Afternoon session lectures
[XY-101]...[XY-199]	Posters

PARALLEL SESSIONS

Analytical Sciences [AS]

Lecture hall G95

Chair: Dr. Hanspeter Andres



Session Endowment: Mettler Toledo

- 11:00 **Pushing the limits of *de novo* genome assembly for complex prokaryotic genomes and establishing a basis to utilize microbiome isolates for plant protection [AS-011]**
Christian Ahrens, Agroscope
- 11:30 **Bioanalytical workflows based on non-target high-resolution mass spectrometry and bioassays for the identification of toxicants in complex water samples [AS-013]**
Tarek Manasfi, Eawag, Dübendorf
C. McArdell*
- 11:45 **Determination of the primary structure of glycans by enzymatic cleavage and cryogenic IR-spectroscopy [AS-014]**
Irina Diukova, EPFL Lausanne
T. Rizzo*
- 12:15 **Magneto-optical Kerr effect set-up for *in situ* probing of oxygen evolution electrodes [AS-016]**
Olga Sambalova, Empa
O. Yildirim, G. R. Patzke, D. Tilley, A. Borgschulte*
- 12:30 **Methane, ammonia and volatile organic compound emissions at herd level in an experimental housing for dairy cows [AS-017]**
Simon Wyss, Empa
S. Schrade, M. Hill, M. Zähler, K. Zeyer, F. Dohme-Meier, S. Reimann, J. Mohn*

Chair: Prof. Stefan Schürch

- 15:00 **The use of UV/VIS spectroscopy in process monitoring and diagnostics [AS-021]**
Hans Joachim Muhr, Mettler-Toledo GmbH
- 15:30 Poster Pitches
- 16:00 **Structure elucidation of low molecular weight compounds in spider venom [AS-025]**
Yvonne Forster, University of Zurich
S. Bienz*, L. Bigler*

- 16:15 **An efficient Autosampler for the Screening of Protein-Ligand Interactions by native ESI-MS [AS-026]**
Jerome Kaeslin, ETH Zurich
R. Zenobi*
- 16:30 **A New ICP-MS Configuration for Single Cell Analysis [AS-027]**
Thomas Vonderach, ETH Zurich
D. Günther*

Catalysis Sciences & Engineering [CE]

Lecture hall G20

Chair: Prof. Jeroen van Bokhoven



Session Endowment: Lonza AG

- 11:00 **Redefining Nucleoside Analog Total Synthesis and Manufacturing [CE-011]**
Louis-Charles Campeau, Merck
- 11:30 **Nature of the synergy between Brønsted and Lewis acid sites in Sn-Beta zeolites for the synthesis of polyoxymethylene dimethyl ethers (OME) [CE-013]**
Christophe Baranowski, EPFL Lausanne
M. Roger, A. Bahmanpour, O. Krocher*
- 11:45 **Understanding the Nature of Surface Sites in Ga₂O₃ Based Catalysts for Propane Dehydrogenation: Acidity, Deactivation, and the Support Effect [CE-014]**
Pedro Castro-Fernández, ETH Zurich
D. Mance, I. B. Moroz, C. Copéret, A. Fedorov, C. R. Müller*
- 12:00 **A Silicon-based Microfluidics Platform for Heterogeneous Catalysis in Wall-coated Flow Reactors [CE-015]**
Dominik Scherrer, University of Basel
U. Drechsler, A. Olziersky, Z. Joncev, D. Miladinov, M. Mayor, C. Sparr*, E. Lörtscher*
- 12:15 **Post-synthesis deposition of mesoporous niobic acid with improved thermal stability by kinetically controlled sol-gel overcoating [CE-016]**
Yuan-Peng Du, EPFL Lausanne
F. Héroguel, J. S. Luterbacher*
- 12:30 **Metal Dependent Structure-Activity Relations in Acetylene Hydrochlorination [CE-017]**
Selina Kaiser, ETH Zurich
R. Lin, G. Manzocchi, J. Pérez-Ramírez*

Chair: Prof. Cristina Nevado

- 15:00 **Process Related Aspects of Industrial Fluorine Chemistry [CE-021]**
Christoph Täschler, Lonza AG
- 15:30 **Structure-activity descriptors for the rational design of materials in direct conversion of methane to methanol [CE-023]**
Vitaly Sushkevich, PSI Villigen
J. A. van Bokhoven*
- 15:45 **Development of a microfluidics-based assay for the evolution of artificial metalloenzymes using a cell surface display strategy [CE-024]**
Jaicy Vallapurackal, University of Basel
A. Stucki, P. Dittrich*, T. Ward*

- 16:00 **Stable and tunable phosphonic acid dipole layer for band edge engineering of photoelectrochemical and photovoltaic heterojunction devices [CE-025]**
Rene Wick-Joliat, University of Zurich
T. Musso, R. R. Prabhakar, S. Siol, W. Cui, J. Löckinger, J. Suh, D. Tilley*
- 16:15 **Active Site Structures in Titanium-Silicalite 1: An NMR Point of View [CE-026]**
Christopher Gordon, ETH Zurich
A. Parvulescu, J. H. Teles, C. Copéret*
- 16:30 **Uncovering the interfacial carrier dynamics in emerging photoelectrodes for solar fuel production – an operando spectroelectrochemical study [CE-027]**
Yongpeng Liu, EPFL Lausanne
K. Sivula, N. Guijarro*

Computational and Theoretical Chemistry [CC]

Lecture hall G85

Chair: Prof. Jeremy Richardson



Session Endowment: Syngenta Crop Protection AG

- 11:00 **In Silico Photochemistry using *Ab Initio* Nonadiabatic Molecular Dynamics [CC-011]**
Basile Curchod, Durham University, UK
- 11:30 **An approach for calculating the logarithmic derivative of the time-dependent wavefunction [CC-013]**
Nikolay Golubev, EPFL Lausanne
- 11:45 **Nonadiabatic molecular dynamics simulations [CC-014]**
Johan Runeson, ETH Zurich
J. O. Richardson*
- 12:00 **Self-consistent DFT+U+V study of oxygen vacancies in SrTiO₃ [CC-015]**
Chiara Ricca, University of Bern
I. Timrov, M. Cococcioni, N. Marzari, U. Aschauer*
- 12:15 **Calculating electronic excitation spectra for large-scale applications [CC-016]**
Anna Hehn, University of Zurich
B. Sertcan, J. Hutter*
- 12:30 **The relationship between physical conditions for ρ_B and the error within Frozen Density Embedding Theory [CC-017]**
Niccolò Ricardi, University of Geneva
A. Zech, Y. Gimbal-Zofka, T. Wesolowski*

Chair: Prof. Marcella Iannuzzi

- 15:00 **Molecular modelling in crop protection: current technologies and applications [CC-021]**
Stefano Rendine, Syngenta Crop Protection AG
- 15:30 **Using RE-EDS to calculate relative binding free energies for ligand scaffold hopping [CC-023]**
Benjamin Schroeder, ETH Zurich
D. Sidler, S. Riniker*
- 15:45 **Molecular Dynamics simulations with RKHS based potentials [CC-024]**
Marco Pezzella, University of Basel
M. Meuwly*

- 16:00 **Automated force-field refinement for compound families [CC-025]**
Marina Pereira Oliveira, ETH Zurich
P. H. Hünenberger*
- 16:15 **Learning (from) the electron density: focus on non-covalent interactions and transferability [CC-026]**
Alberto Fabrizio, EPFL Lausanne
A. Grisafi, B. Meyer, M. Ceriotti, C. Corminboeuf*
- 16:30 **Alchemical Perturbation Density Functional Theory (APDFT) [CC-027]**
Guido Falk von Rudorff, University of Basel
O. A. von Lilienfeld*

Inorganic & Coordination Chemistry [IC]

Lecture hall G30

Chair: Prof. Marinella Mazzanti



Session Endowment: Clariant International Ltd.

- 11:00 **Electrochemical and Photochemical Transformations of Dinitrogen [IC-011]**
Sven Schneider, Georg-August-Universität Göttingen
- 11:30 **Addressing Lattice Flexibility in Metal Organic Framework Membranes for Carbon Capture [IC-013]**
Deepu Babu, EPFL Lausanne
K. V. Agrawal*
- 11:45 **100-fold Increase in Colloidal Stability of Cesium Lead Halide Perovskite Nanocrystals using Lecithin as Capping Ligand [IC-014]**
Franziska Krieg, ETH Zurich
M. V. Kovalenko*
- 12:00 **Chemistry at High Dilution: Dinuclear ^{99m}Tc complexes do exist! [IC-015]**
Robin Bolliger, University of Zurich
H. Braband, G. Meola, R. Alberto*
- 12:15 **Bimetallic Dirhodium Complexes as Models to Study Hydrogen Activation on Carbon-Supported Rh(0) Catalysts [IC-016]**
Pascal Jurt, ETH Zurich
T. L. Gianetti, A. Fedorov, H. Grützmacher*
- 12:30 **Quantitative insights into charge-separated states relevant for artificial photosynthesis [IC-017]**
Svenja Neumann, University of Basel
C. Kerzig*, O. S. Wenger*

Chair: Prof. Kay Severin

- 15:00 **Enhanced charge carrier transport in sulfurized Sb₂Se₃ investigated by in-situ potential sensing and time-resolved spectroscopy [IC-021]**
Rajiv Prabhakar, University of Zurich
T. Moehl, D. Fiedrich, W. Cui, D. Tilley*
- 15:15 **A new post-synthetic polymerization strategy makes metal-organic frameworks more stable [IC-022]**
Shuliang Yang, EPFL Lausanne
L. Peng, D. T. Sun, M. Asgari, E. Oveisi, O. Trukhina, S. Bulut, A. Jamali, W. L. Queen*

- 15:30 **Manganese(II)-Catalyzed Asymmetric Hydrogenation of Ketones: Exploring the Analogy to Iron(II) [IC-023]**
Alessandro Passera, ETH Zurich
A. Mezzetti*
- 15:45 **Nickel complexes containing oxygen-chelating mesoionic carbenes as easily accessible catalysts for CO₂ reduction [IC-024]**
Simone Bertini, University of Bern
M. Rahaman, F. Gloaguen, P. Schollhammer, P. Broekmann, M. Albrecht*
- 16:00 **Tuning Reactivity of Nitride Bridged Uranium Complexes with Amide and Siloxide Ligands [IC-025]**
Chad Palumbo, EPFL Lausanne
L. Barluzzi, R. Scopelliti, M. Mazzanti*
- 16:15 **Proximal Monomeric Cu(II) Sites on Alumina Convert Selectively CH₄ to CH₃OH [IC-026]**
Jordan Meyet, ETH Zurich
K. Searles, M. Newton, A. P. van Bavel, A. D. Horton, J. A. van Bokhoven*, C. Copéret*
- 16:30 **A Novel Ni-containing B₁₂ Derivative – Elucidating the Origin of Corrinoid and Corphinoid Cofactors [IC-027]**
Christopher Brenig, University of Zurich
L. Prieto, R. Oetterli, F. Zelder*

Medicinal Chemistry & Chemical Biology [MC]

Lecture hall G60

Chair: Prof. Jean-Louis Reymond



Session Endowment: Idorsia Pharmaceuticals Ltd

- 11:00 **DMCCB General Assembly [MC-011]**
Jean-Louis Reymond, University of Bern
- 11:15 **Photoactivation of silicon rhodamines via a light-induced protonation [MC-012]**
Michelle Frei, EPFL Lausanne and Max Planck Institute for Medical Research
L. Reymond*, K. Johnsson*
- 11:30 **Discovery of potent CXCR3 antagonists with therapeutic potential in autoimmune diseases [MC-013]**
Eva Caroff, Idorsia Pharmaceuticals Ltd.
E. Meyer, H. Siendt, T. Kimmerlin, P. Äanismaa, N. Schmitz, M. Keller*
- 11:45 **Structural insights into molecular oxygen binding and activation by formylglycine generating enzyme [MC-014]**
Dzmitry Miarzlou, University of Basel
F. Leisinger, D. Joss, D. Häussinger*, F. P. Seebeck*
- 12:00 **Discovery and optimization of novel, potent mGlu4 NAM compounds [MC-015]**
Fionn O'Hara, F. Hoffmann-La Roche Ltd
L. Gobbi, M. Honer, L. Lindemann, D. Muri, S. Pichereu, J.-M. Plancher, B. Biemans*, G. Jaeschke*
- 12:15 **Polymerase Amplification-Mass Spectrometry Coupled Quantitation of a Mutagenic DNA Adduct [MC-016]**
Claudia Aloisi, ETH Zurich
A. Nilforoushan, N. Ziegler, S. J. Sturla*
- 12:30 **LMW VAV1 Inhibitors: Discovery, Optimization, & Mode of Action Studies [MC-017]**
Philip Skaanderup, Novartis Pharma AG

Chair: Dr. Fides Benfatti

- 15:00 **C-terminal Bioconjugation Through Photoredox Catalyzed Decarboxylative Alkynylation [MC-021]**
Marion Garreau, EPFL Lausanne
F. Le Vaillant, J. Waser*
- 15:15 **Stabilizing inactive conformations of MALT1 as an effective strategy to inhibit its protease activity [MC-022]**
Jean-Baptiste Langlois, Novartis Pharma AG
P. Erbel, N. Aubin, F. Bornancin, C. Wiesmann, F. Villard, B. Gerrits, J. Quancard, A. Schlapbach, J. Langlois*, M. Renatus*
- 15:30 **A nanotechnological approach to synthetic biology: cascade reactions in synthetic compartments [MC-023]**
Andrea Belluati, University of Basel
A. Belluati, J. Liu, S. Thamboo, C. G. Palivan*
- 15:45 **From Setipiprant to ACT-774312: discovery of new potent CRTH2 antagonists [MC-024]**
Romain Siegrist, Idorsia Pharmaceuticals Ltd.
M. Holdnener, P. Bouis, C. Gnerre, J. Hazemann, S. Richard, C. Boss, H. Aissaoui*
- 16:00 **Synthesis of new aminopyrazole analogues with promising anti-leishmaniosis activity: A University-DNDi Open Synthesis Project [MC-025]**
Sébastien Tardy, University of Geneva
Students from BUSP2, C. Cecchini, H. M. Ismail, N. Deschamps, L. Pellissier, A. Rutz, M. Fu, E. Varesio, L. Scapozza*, B. Perry*
- 16:15 **Discovery and optimisation of novel compounds for malaria vector control [MC-026]**
Ottmar Hueter, Syngenta Crop Protection AG
M. Hoppé, P. Wege, R. Nourani, M. Daniels, P. Maienfisch
- 16:30 **Advanced building blocks for medicinal chemistry from the chemical universe database GDB [MC-027]**
Kris Meier, University of Bern
J.-L. Reymond*

Organic Chemistry [OC]

Lecture hall G45

Chair: Prof. Jason Holland



Session Endowment: Janssen R&D / Cilag AG

- 11:00 **Harnessing Nature's Toolbox for Selective Halogenations: New Concepts for an Old Problem [OC-011]**
Tanja Gulder, Technical University Munich
- 11:30 **Facile Access to Nitroarenes and Nitroheteroarenes Using N-Nitrosaccharin: An Electrophilic Nitrating Reagent [OC-013]**
Roxan Calvo, ETH Zurich
K. Zhang, A. Passera, D. Katayev*
- 11:45 **Novel 'migratory' C(sp²)-C(sp) reductive elimination on Gold(III) complexes: a mechanistic insight [OC-014]**
Alexandre Genoux, University of Zurich
J. González, E. Merino, C. Nevado*
- 12:00 **Studies towards the Synthesis of Shearinine Natural Products [OC-015]**
Nicole Hauser, ETH Zurich
M. A. Imhof, E. M. Carreira*

- 12:15 **Enantioselective Nickel-Catalyzed Amination of 2-Substituted 1,3-Dienes [OC-016]**
Gaël Tran, University of Geneva
W. Shao, C. Mazet*
- 12:30 **Pd⁰-Catalyzed C(sp³)-H Activation: From Direct to Remote Functionalization for the Construction of Medium-Sized Rings [OC-017]**
Ronan Rocaboy, University of Basel
O. Baudoin*

Chair: Prof. Pablo Rivera-Fuentes

- 15:00 **Asymmetric Synthesis of Esketamine [OC-021]**
Cheng Yi Chen, Janssen R&D / Cilag AG
- 15:30 **Preparation of Indolenines via Nucleophilic Aromatic Substitution [OC-023]**
Joel Roesslein, University of Zurich
F. Huber, K. Gademann*
- 15:45 **Chiral Cyclopentadienyl Ligands: Structural Insights and Application in Enantioselective Cyclopropanation [OC-024]**
Coralie Duchemin, EPFL Lausanne
N. Cramer*
- 16:00 **Stereodivergent Catalyst Control of Two Stereogenic Axes [OC-025]**
Daniel Moser, University of Basel
C. Sparr*
- 16:15 **Reactivity and synthetic utility of a-boryl carbon centered radicals: two opposing reaction manifolds [OC-026]**
Nicholas Tappin, University of Bern
W. Michalska, S. Rohrbach, M. Gnaegi-Lux, P. Renaud*
- 16:30 **A Tethered Approach to the Palladium Catalyzed Dual Functionalization of Alkynes [OC-027]**
Phillip Greenwood, EPFL Lausanne
E. Grenet, J. Waser*

Physical Chemistry [PC]

Lecture hall G40

Chair: Dr. Arianna Marchionne

Siegfried

Session Endowment: Siegfried AG

- 11:00 **Many-body elastic scattering of exciton polarons in organic-inorganic hybrid perovskites [PC-011]**
Carlos Silva, Georgia Institute of Technology, USA
- 11:30 **Hot Carrier Dynamics in Lead Halide Perovskites from a THz Mobility Perspective [PC-013]**
Andrés Burgos-Caminal, EPFL Lausanne
A. Willauer, J. M. Moreno-Naranjo, A. Ajdar-Zadeh, J.-E. Moser*
- 11:45 **Underestimated Effect of a Polymer Matrix on the Light Emission of Single CsPbBr₃ Nanocrystals [PC-014]**
Gabriele Ràino, ETH Zurich
A. Landuyt, F. Krieg, C. Bernasconi, S. Ochsenbein, D. N. Dirin, M. Bodnarchuk, M. V. Kovalenko*
- 12:00 **What determines the open circuit voltage of Perovskite solar cells? [PC-015]**
Nikolaos Drosos, University of Bern
D. Tsokkou, V. Brehm, P. Boix, H. J. Bolink, N. Banerji*

- 12:15 **Bulk hyperpolarization of inorganic materials [PC-016]**
Snædís Björgvinsdóttir, EPFL Lausanne
B. J. Walder, P. Moutzouri, N. Matthey, L. Emsley*
- 12:30 **Towards time-resolved laser T-jump/X-ray absorption probe spectroscopy [PC-017]**
Oliviero Cannelli, EPFL Lausanne
C. Bacellar, R. A. Ingle, R. Bohinc, D. Kinschel, D. Ferreira Sanchez, D. Grolimund, G. F. Mancini*, M. Chergui*

Chair: Dr. Tatu Kumpulainen

- 15:00 **Structural Dynamics of an Excited Donor-Acceptor Complex: Ultrafast Polarized Infrared Spectroscopy and Mixed Quantum/Classical Simulations [PC-021]**
Christopher Rumble, University of Geneva
E. Vauthey*
- 15:15 **Signatures of intra-/intermolecular vibrational coupling in halogenated liquids revealed by 2D Raman-THz spectroscopy [PC-022]**
Gustavo Ciardi, University of Zurich
A. Berger, A. Shalit, P. Hamm*
- 15:30 **Solvation in a Propyl Acetate/Butyronitrile Mixture [PC-023]**
Pragya Verma, University of Geneva
T. Kumpulainen*
- 15:45 **Using IRPD-spectroscopy for onium ions serving as a molecular balance for the estimation of non-covalent interactions [PC-024]**
Vladimir Gorbachev, ETH Zurich
A. Tsybizova, L. Fritsche, L. Miloglyadova, P. Chen*
- 16:00 **Photochemistry of single optically trapped organic aerosol droplets: The photodegradation of oleic acid by oxygen [PC-025]**
Evelyne Parmentier, ETH Zurich
G. David, P. Corral Arroyo, S. Bibawi, R. Signorell*
- 16:15 **High Resolution Infrared Spectroscopy of Monodeuterated Ethylene Oxide $c\text{-C}_2\text{D}_3\text{O}$: Analysis of the Infrared Spectrum of several Ring Deformation and Stretching Fundamentals [PC-026]**
Karen Keppler, ETH Zurich
S. Albert, Z. Chen, C. Manca Tanner, V. Schurig, J. Stohner, O. Trapp, M. Quack*
- 16:30 **Reaction kinetics of trapped molecular ions with conformer- and isomer-selected neutral molecules [PC-027]**
Ardita Kilaj, University of Basel
H. Gao, D. Rösch, U. Rivero, S. Willitsch*, J. Küpper*

Polymers, Colloids & Interfaces [PI]

Lecture hall G55

Chair: Prof. Walter Remo Caseri



- Session Endowment: Dow Europe GmbH
- 11:00 **The evolution of polymer chemistry in the preservation of monuments [PI-011]**
Maria Laura Santarelli, University of Rome Sapienza
M. P. Bracciale
- 11:30 **Host-guest interactions on electrode surfaces for immobilization of molecular catalysts [PI-013]**
Laurent Severy, University of Zurich
J. Szczerbinski, M. Iannuzzi, G. Tocci, R. Zenobi, D. Tilley*
- 11:45 **Carbon Nanomaterial Formation at the Liquid-Liquid Interface [PI-014]**
Enzo Bomal, EPFL Lausanne
R. Yeo, N. Candau, H. Frauenrath*
- 12:00 **The interplay of channel geometry and molecular features determine diffusion in lipidic cubic phases [PI-015]**
Reza Ghanbari, Adolphe Merkle Institute / University of Fribourg
R. Mezzenga
- 12:15 **Performance at Interfaces – from hair to ceramic tiles [PI-016]**
Dirk Kuppert, Clariant

Chair: Dr. Dominik Brühwiler

- 15:00 **EPDM Rubber Developments Enabled By Advanced Molecular Catalyst Technology [PI-021]**
Varun Thakur, Dow Europe GmbH
S. Wu, C. L. P. Shan, V. Thakur*
- 15:30 **Polymer Brush Functionalized Magnetic Nanoparticle Clusters as Magnetic Blood Purification Agents [PI-023]**
Alexandre Anthis, Empa
M. T. Matter, I. K. Herrmann*
- 15:45 **3D Printing of Personalized Biodegradable Airway Stents via Vat Photopolymerization [PI-024]**
Yinyin Bao, ETH Zurich
K. Masania, N. Kleger, J. Cadalbert, J. Leroux*
- 16:00 **Developing A Safe by Design Nanoagrochemical [PI-025]**
Fabienne Schwab, University of Fribourg
M. Maceroni, M. H. El-Shetehy, L. Ackermann-Hirschi, A. Moradi, F. Mauch, B. Rothen-Rutishauser, A. Petri-Fink, F. Schwab*
- 16:15 **Amine functionalized nanofiber aerogel for efficient CO₂ capture [PI-026]**
Sara Mousavi, Zurich University of Applied Sciences ZHAW
S. Ko, C. Adlhart*
- 16:30 **Mechanochemical Activation at Interfaces Driven by Swelling of Polymer Brushes [PI-027]**
Julian Bleich, EPFL Lausanne
M. M. Marcinek, H. A. Klok*

POSTER SESSIONS

Poster Presentation Title [Code]

First line = Presenting Author, Affiliation

Second line = Co-authors

* Research Head(s)

Analytical Sciences [AS] Poster Session

Ultrahigh ion-mobility separation of CID fragments for glycan analysis [AS-101]

Priyanka Bansal, EPFL Lausanne
A. Ben Faleh, S. Warnke, T. Rizzo*

Efficient Tip Recycling for AFM-based Tip-Enhanced Raman Spectroscopy (TERS) [AS-102]

Giovanni Bartolomeo, ETH Zurich
A. K. Sachan, G. Goubert, R. Zenobi*

Mass spectrometric investigation of neutral soluble dietary fiber interactions with small molecules [AS-103]

Samy Boulos, ETH Zurich
L. Nyström*

Host-guest interaction to improve the bioavailability of bent metallocenes? A mass spectrometric investigation [AS-104]

Pia Bruni, University of Bern
S. Schürch*

A laser ablation ionization mass spectrometry approach for compositional analysis of Sn/Ag solder bumps [AS-105]

Alena Cedeño López, University of Bern
V. Grimaudo, A. Riedo, M. Tulej, R. Wiesendanger, R. Lukmanov, P. Moreno-García, P. Wurz*, P. Broekmann*

The Transfer Rate of PCBs from Feed to Adipose Tissue Depends on Body Fatness in Growing Cattle [AS-106]

Charlotte Driesen, Empa
I. Morel, H. D. Hess, M. Zennegg*, S. Lerch*

Chemical Characterization of Proteo-lipidic Membranes with Atomic Force Microscopy and Tip-Enhanced Raman Spectroscopy [AS-107]

Guillaume Goubert, ETH Zurich
A. K. Sachan, R. Zenobi*

Novel strategies using UV and IR fs-LIMS for chemical depth profiling in laboratory space application [AS-108]

Valentine Grimaudo, University of Bern
A. Riedo, A. Cedeño López, M. Tulej, P. Broekmann, P. Wurz*

The A2[3]G1 and A2[6]G1 N-glycan structures by ion mobility mass spectrometry [AS-109]

Joanna Hajduk, ETH Zurich
A. Marchand, M. F. Czár, R. Zenobi*

Capabilities of Single Particle Inductively Coupled Plasma Mass Spectrometry using different sample introduction strategies [AS-110]

Jovana Kocic, ETH Zurich
D. Günther, B. Hattendorf*

Characterizing iron loading pattern of ferritin through native MS [AS-111]

Jiayi Lan, ETH Zurich
R. Zenobi*

Nanoparticles tethered polysaccharide probes for potential investigation of supramolecular interactions between water soluble dietary fiber and target compounds. [AS-112]

Cristina Lupo, ETH Zurich
S. Boulos, L. Nyström*

Pesticide multi residue LCMS analysis for soil monitoring within the action plan plant protection products [AS-113]

Simon Mangold, Agroscope
F. Wettstein, T. Bucheli

Concurrency analysis: a tool for discovery of multi-elemental nanoparticles measured with single-particle ICP-TOFMS [AS-114]

Kamyar Mehrabi, ETH Zurich
D. Günther, A. Gundlach-Graham*

Conformational studies on desolvated biomolecules [AS-115]

Jonas Metternich, ETH Zurich
A. Marchand, M. F. Czár, P. Tiwari, Y. Fleischmann, R. Zenobi*

Modelling archaeological wood degradation and validation by chemometry [AS-116]

Mathilde Monachon, University of Neuchatel
M. Albelda Berenguer, E. Joseph

Methods to improve resolution in ¹H solid state NMR at ultra-fast MAS [AS-117]

Pinelopi Moutzouri, EPFL Lausanne
F. M. Paruzzo, L. Emsley*

Tip-enhanced Raman Spectroscopy on Two-Dimensional Polymers and Chemically Functionalized Surfaces [AS-118]

Timo Niepel, ETH Zurich
R. Zenobi*

Microwave Inductively Coupled Nitrogen Plasma Quadrupole Mass Spectrometry [AS-119]

Mohammad I. Nouraddini, ETH Zurich
J. Jevtic, A. Menon, D. Günther, B. Hattendorf*

Metabolism During Sleep Monitored by Real-Time Breath Analysis [AS-120]

Nora Nowak, ETH Zurich
T. Gaisl, M. Osswald, D. Miladinovic, S. Bauer, J. Buhmann, M. Kohler, P. M. L. Sinues, R. Zenobi*, S. Brown*

In situ Tip-Enhanced Raman Spectroscopy of 2D materials [AS-121]

Yashashwa Pandey, ETH Zurich
J. Szczerbinski, G. Goubert, R. Zenobi*

Thermal Denaturation of G-quadruplexes and Their Effects on the Stability of Adjacent DNA Duplexes Studied by Temperature-Controlled nanoESI-MS [AS-122]

Adam Pruška, ETH Zurich
A. Marchand, R. Zenobi*

Direct Laser Desorption Mass Spectrometry of Amino Acids on Ocean Worlds [AS-123]

Andreas Riedo, Leiden University
N. Ligterink, V. Grimaudo, P. Moreno-García, R. Wiesendanger, R. Lukmanov, M. Tulej, R. Lindner, P. Wurz, P. Ehrenfreund*

Investigation of Corneal Crosslinks in Keratoconus Treatment [AS-124]

Nina Röthlisberger, University of Bern
M. Ariza, P. Büchler, S. Schürch*

POPs in microplastics in the South Atlantic gyre and their environmental risks [AS-125]

Lena Schinkel, Empa
L. Amaral-Zettler, E. Zettler, P. Delandmeter, F. A. de Vogel, E. Edson, H. Limburg, V. Onink, N. Heeb, M. Zennegg*

Deep UV Raman spectroscopy for online water analysis [AS-126]

Andrea Sterzi, Empa
U. Schneider, O. Sambalova, D. Bleiner, A. Borgschulte*

Standardization procedure for exhaled breath analysis using secondary electrospray ionization mass spectrometry [AS-127]

Bettina Streckenbach, ETH Zurich
N. Perkins, S. Mueller, T. Bruderer, A. Moeller*, R. Zenobi*

LC-APCI(-)-MS analysis of 1-chloro-2,4-dinitrobenzene, a model substrate for glutathione S-transferases [AS-128]

Marc J-F Suter, Eawag, Dübendorf
A. Tierbach, K. J. Groh, R. Schönenberger, K. Schirmer

Comparison of SIM Stitch and full mass scan direct infusion metabolomics for the assessment of the molecular stress response in *Chlamydomonas reinhardtii* exposed to Ag²⁺ [AS-129]

Marc J-F Suter, Eawag, Dübendorf
S. Salzmann

Gas-phase fluorescence from trapped biomolecular ions: instrumentation and photophysical studies [AS-130]

Prince Tiwari, ETH Zurich
J. B. Metternich, M. F. Czár, R. Zenobi*

Quantitative microanalysis of porous materials by means of Laser Ablation Plasma Mass Spectrometry [AS-131]

Adrian Wichser, Empa Dübendorf
M. Trottmann, J. Niederberger, D. Bleiner*

Investigation of neutral soluble dietary fibre interactions with nutritional molecules and mineral cations by electron paramagnetic resonance spectroscopy [AS-132]

Xiaowen Wu, ETH Zurich
V. Syryamina, S. Boulous, M. Yullikov, L. Nyström*

Trapped ions accelerate the crystallization of amorphous calcium carbonate in air [AS-133]

Jacinta Xto, Paul Scherrer Institute, Villigen
C. Borca, J. A. van Bokhoven, T. Huthwelker

A Disassembly Approach for Selective Detection of Pyrophosphate using Fe^{III}-Salen Complexes [AS-134]

Prerna Yadav, University of Zurich
M. Jakubaszek, G. Gasser, F. Zelder*

N-glycan analysis with ultrahigh-resolution ion mobility spectrometry and cryogenic ion spectroscopy [AS-135]

Natalia Yalovenko, EPFL Lausanne
A. Ben Faleh, S. Warnke, T. Rizzo*

Time trends of persistent organic pollutants in Swiss human milk samples [AS-136]

Markus Zennegg, Empa
T. Känzig, A. Buser, J. Tremp, C. Cripe, A. Genewein, D. Bleiner*

Modern X-ray spectroscopy: XAFS and XES in the Laboratory [AS-137]

Patric Zimmermann, ETH Zurich
P. M. Abdala, C. R. Müller, J. A. van Bokhoven*

Catalysis Sciences & Engineering [CE] Poster Session**Aging of Model Diesel Oxidation Catalysts: Hydrothermal vs Chemical Effects [CE-101]**

Miren Agote-Arán, Paul Scherrer Institute, Villigen
C. Coffano, O. Krocher, D. Ferri*

Exsolution of Metallic Ru Nanoparticles to Impart Stability on Catalysts for the Dry Reforming of Methane [CE-102]

Muhammad Awais Naeem, ETH Zurich
P. M. Abdala, A. Fedorov, C. R. Müller*

In-situ formed highly stable Cu-Al catalyst for the Reverse Water Gas Shift reaction [CE-103]

Ali Bahmanpour, EPFL Lausanne
F. Héroguel, C. Baranowski, L. Artiglia, J. S. Luterbacher, U. Röthlisberger, M. Kilic, O. Krocher*

Electrochemical stability and mechanistic studies of mixed oxides upon water oxidation investigated by *in situ* electrochemical XAS [CE-104]

S. Balaghi, University of Zurich
G. R. Patzke*

In situ spatial resolution in catalysis [CE-105]

Arik Beck, ETH Zurich
X. Huang, M. Zabilskiy, L. Artiglia, M. G. Willinger*, J. A. van Bokhoven*

Hydrogen on Cu/ZnO catalysts [CE-106]

Andreas Borgschulte, Empa
J. Terreni, O. Sambalova, P. Trtik

Selectivity Descriptors for Nickel Catalysts based on Tailored Carbons in the Electroreduction of CO₂ [CE-107]

Simon Büchele, ETH Zurich
A. J. Martin, S. Mitchell, J. Pérez-Ramírez*

Metal-Organic Frameworks for Catalysis: a systematic study of their stability [CE-108]

Daniele Cartagenova, Paul Scherrer Institute, Villigen
F. A. Peixoto Esteves, J. A. van Bokhoven, M. Ranocchiaro*

N-heterocycles for Hydrogen Storage and Delivery using Homogeneous Ruthenium(II) Phosphine Catalysts [CE-109]

Lu Chen, EPFL Lausanne
P. J. Dyson*, G. Laurency*

Screening Alkaline Earth Metal Catalysts for Hydrogenation of Alkenes using Molecular Volcano Plots [CE-110]

Shubhajt Das, EPFL Lausanne
C. Corminboeuf*

Noncovalent Interactions Drive the Efficiency of Mo Imido Alkylidene Catalysts for Olefin Metathesis [CE-111]

Jordan De Jesus Silva, ETH Zurich
M. A. Ferreira, S. Grosslight, A. Fedorov, M. S. Sigman, C. Copéret*

Exploring the role of secondary metals in the selective hydrogenation of CO₂ at supported palladium nanoparticles – an SOMC approach [CE-112]

Scott Docherty, ETH Zurich
C. Copéret*

Atomic-Scale Engineering of Indium Oxide Promotion by Palladium for Maximized and Stable Methanol Production via CO₂ Hydrogenation [CE-113]

Matthias Frei, ETH Zurich
C. Mondelli, R. García-Muelas, K. K. Kley, B. Puértolas, N. López, O. V. Safonova, J. A. Stewart, D. Curulla Ferré, J. Pérez-Ramírez*

Superior performances of Fe-FER compare to Fe-ZSM5 in NO_x and N₂O abatements [CE-114]

Alberto Garbujo, CASALE SA
R. Lanza, E. Rohart, A. Lahougue, G. Gaudry, R. Ostuni, P. Biasi*

Fabrication and *in situ* heating TEM studies of a recyclable manganese oxide based anode for water oxidation [CE-116]

Sima Heidari, University of Zurich
A. Sologubenko, G. R. Patzke*

Biogas from microbial electrolysis [CE-117]

Marion Jaussi, HES-SO Valais-Wallis
C. P. Cachelin, F. Fischer*

Efficient reductive amination of HMF with well-dispersed Pd nanoparticles immobilized in a porous MOF/polymer composite [CE-118]

Vikram Karve, EPFL Valais Wallis, Sion
D. T. Sun, O. Trukhina, S. Yang, E. Oveisi, J. S. Luterbacher, W. L. Queen*

Sorption-enhanced steam methane reforming over Ru/Ca₃Al₂O₆-CaO bi-functional catalyst-CO₂ sorbent for the production of high purity hydrogen [CE-119]

Sung Min Kim, ETH Zurich
P. M. Abdala, D. Hosseini, A. Armutlulu, T. Margossian, C. R. Müller*

Copper-exchanged omega (MAZ) zeolite: morphology dependent conversion of methane to methanol [CE-120]

Amy Knorpp, ETH Zurich
A. B. Pinar, M. Newton, J. A. van Bokhoven*

Ru-modified zeolite catalyzed indirect CO₂ methanation: Hydrogenolysis of cyclic carbonates [CE-121]

Wei Tse Lee, EPFL Lausanne
P. J. Dyson*

The activity of single atoms and particles in steam-treated Pt/CeO₂ catalyst studied with *in situ* ambient X-ray photoelectron spectroscopy [CE-122]

Xiansheng Li, Paul Scherrer Institute, Villigen
L. Artiglia*, J. A. van Bokhoven*

Dynamic role of molecular cocatalysts on hematite photoanodes for water oxidation [CE-123]

Jingguo Li, University of Zurich
G. R. Patzke*

Uncovering the interfacial carrier dynamics in emerging photoelectrodes for solar fuel production – an operando spectroelectrochemical study [CE-124]

Yongpeng Liu, EPFL Lausanne
K. Sivula, N. Guijarro*

Impact of Carrier Acidity on the Conversion of Syngas to Higher Alcohols over Zeolite-Supported Copper-Iron Catalysts [CE-125]

Ho Ting Luk, ETH Zurich
C. Mondelli, J. A. Stewart, D. Curulla Ferré, J. Pérez-Ramírez*

Revising the mechanism of the catalytic ethanol oxidation [CE-126]

Sotiria Mostrou, ETH Zurich
N. Nagl, K. Föttinger, J. A. van Bokhoven*

Defect-induced enhanced activity in Ce-substituted La_{0.6}Sr_{0.4}MnO_{3±δ}, a promising perovskite redox material class for solar thermochemical CO₂ splitting [CE-127]

J. Madhusudhan Naik, University of Zurich
A. Steinfeld, G. R. Patzke*

Generation and understanding of low-valent Molybdenum sites towards olefin metathesis [CE-128]

Darryl Nater, ETH Zurich
N. Kaeffer, C. Copéret*

Modulated-Excitation Spectroscopy of Cu/SSZ-13: Unraveling the Mechanism of Selective Catalytic Reduction (SCR) [CE-129]

Rob Jeremiah Nuguid, Paul Scherrer Institute, Villigen
A. H. Clark, M. Nachtegaal, D. Ferri, O. Kroecher*

Halogen-Mediated Valorization of Methane over Zeolites: Interaction of Halogenated Compounds with MFI [CE-130]

Vladimir Paunović, ETH Zurich
S. Mitchell, J. Pérez-Ramírez*

Heterogeneous Olefin Metathesis Catalysts prepared via SOMC: which metal, which ligand for which olefins [CE-131]

Margherita Pucino, ETH Zurich
C. P. Gordon, C. Copéret*

Fast Pyrolysis of Lignin Model Compounds [CE-132]

Allen Puente-Urbina, ETH Zurich
R. Haaring, Z. Pan, P. Hemberger, J. A. van Bokhoven*

Lignin Stabilization to Improve Fast Pyrolysis [CE-133]

Allen Puente-Urbina, ETH Zurich
A. Singh-Morgan, J. S. Luterbacher, J. A. van Bokhoven*

Evolution of Pore Networks in the Synthesis and Catalytic Application of Hierarchical MFI Zeolites [CE-134]

Begoña Puértolas, ETH Zurich
L. Gerchow, P. Crivelli, J. Kenvin, S. Mitchell*, J. Pérez-Ramírez*

Trends and advances in the selective partial oxidation of methane [CE-135]

Manoj Ravi, ETH Zurich
J. A. van Bokhoven*

Development of a Heterogeneous Pt/Zn Catalyst for Propane Dehydrogenation from Surface Organometallic Chemistry Principles [CE-136]

Lukas Rochlitz, ETH Zurich
C. Copéret*

Polyol synthesis route of ceria/zirconia oxides for methane oxidation under stoichiometric conditions [CE-137]

Maneka Roger, EPFL Lausanne
A. Testino, O. Krocher*, D. Ferri*

Epitaxially-Directed Iridium Nanostructures on Rutile-Type Carriers for the Selective Catalytic Hydrodechlorination of Dichloromethane [CE-138]

Ali Saadun, ETH Zurich
G. Zichittella, V. Paunović, B. A. Markaide-Aiastui, S. Mitchell, J. Pérez-Ramírez*

Mechanism of preferential carbon monoxide oxidation on supported Pt-Fe catalysts [CE-139]

Iliya Sadykov, Paul Scherrer Institute, Villigen
M. Zabilskiy, J. A. van Bokhoven, O. V. Safonova*, O. V. Safonova*

Pyridylidene Amide Ligands for Highly Efficient Olefin Oxidation [CE-140]

Kevin Salzmann, University of Bern
C. Segarra, M. Albrecht*

Mining the C–C Cross-Coupling Genome using Machine Learning [CE-141]

Boodsarin Sawatlon, EPFL Lausanne
M. D. Wodrich, B. Meyer, A. Fabrizio, C. Corminboeuf*

Anhydrous conditions enable the catalyst-free carboxylation of alkynes with CO₂ under ambient conditions [CE-142]

Davide Toniolo, EPFL Lausanne
F. Bobbink, M. Mazzanti*, P. J. Dyson*

Evidences and Conjectures on the Initiation Process in Cr-based ethylene polymerization [CE-143]

David Trummer, ETH Zurich
F. Allouche, K. Searles, R. A. Andersen, C. Copéret*

Development of a microfluidics-based assay for the evolution of artificial metalloenzymes using a cell surface display strategy [CE-144]

Jaicy Vallapurackal, University of Basel
A. Stucki, P. Dittrich*, T. Ward*

Nitride-Derived Copper Modified with Indium as a Highly Stable and Selective Catalyst for the Electroreduction of CO₂ [CE-145]

Florentine Veenstra, ETH Zurich
A. J. Martín, J. Pérez-Ramírez*

Atom-by-Atom Resolution of Structure-Function Relations over Low-Nuclearity Metal Catalysts [CE-147]

Evgeniya Vorobyeva, ETH Zurich
E. Fako, Z. Chen, N. López, O. V. Safonova, S. Mitchell*, J. Pérez-Ramírez*

Transition metal electrocatalysts encapsulated into N-doped carbon nanotubes on graphene nanosheets: Efficient water splitting through synergistic effects [CE-148]

Wenchao Wan, University of Zurich
J. R. Li, C. A. Triana, G. R. Patzke*

Stability of atomically dispersed platinum catalysts on low index and stepped CeO₂ surface from density functional theory [CE-149]

Xing Wang, ETH Zurich
J. A. van Bokhoven*, D. Palagin*

On the photoionization of the vinyl radical [CE-150]

Xiangkun Wu, Paul Scherrer Institute, Villigen
P. Hemberger, X. Zhou*, A. Bodi*

Revising the mechanism of alcohol oxidation over V₂O₅/TiO₂ catalysts [CE-151]

Anna Zabilska, Paul Scherrer Institute, Villigen
A. H. Clark, O. Kroecher, O. V. Safonova*

The role of copper-zinc alloy in catalytic carbon dioxide hydrogenation to methanol [CE-152]

Maxim Zabilskiy, Paul Scherrer Institute, Villigen
V. L. Sushkevich, D. Palagin, M. Newton, F. Krumeich, M. Zabilskiy*, J. A. van Bokhoven*

ZnO-Based Catalysts through Atomic Layer Deposition for CO₂ Hydrogenation to Methanol [CE-153]

Ming-Ming Wang, EPFL Lausanne
M. Wang, S. Kim, A. Tsoukalou, Y. Xu, P. M. Abdala, A. Fedorov*, C. R. Müller*

Direct Conversion of Methane to Methanol over Cu-Erionite Zeolite [CE-154]

Jie Zhu, ETH Zurich
V. L. Sushkevich, A. J. Knorpp, M. Newton, S. C. Mizuno, T. Wakihara, T. Okubo, Z. Liu, J. A. van Bokhoven*

Designer 3D Yolk@Shell TiO_{2-x}/LDH Architecture for Powerful Visible Light CO₂ Conversion [CE-155]

Abolfazl Ziarati, University of Geneva
T. Bürgi*

Selective Propylene Production via Propane Oxidation on Metal Phosphate Catalysts [CE-156]

Guido Zichittella, ETH Zurich
G. Stähelin, F. M. Goedicke, J. Pérez-Ramírez*

Computational and Theoretical Chemistry [CC] Poster Session**DDT – Drug Discovery Tool: a fast and intuitive graphics user interface for Docking and Molecular Dynamics analysis [CC-101]**

Simone Aureli, Università della Svizzera italiana
V. Limongelli*

Single-Hessian thawed Gaussian approximation: The missing rung on the ladder [CC-102]

Tomislav Begusic, EPFL Lausanne
M. Cordova, J. Vanicek*

Real-Time Spectroscopy in an Interactive Quantum Chemistry Framework [CC-103]

Francesco Bosia, ETH Zurich
T. Weymuth, A. C. Vaucher, M. Reiher*

Self-Parametrizing System-Focused Models [CC-104]

Christoph Brunken, ETH Zurich
M. Reiher*

Implementation of linear-response TDDFT for X-Ray absorption spectroscopy in CP2K [CC-105]

Augustin Bussy, University of Zurich
M. Iannuzzi, J. Hutter

Efficient geometric integrators for nonadiabatic quantum dynamics in the adiabatic representation [CC-106]

Seonghoon Choi, EPFL Lausanne
J. Vanicek*

An atomistic view over Mg²⁺ induced kinetic heterogeneity in the group II intron-exon recognition site [CC-107]

Richard Cunha, University of Zurich
R. K. O. Sigel*

Analytical implementation of atomic polar tensors in CP2K [CC-108]

Edward Ditler, University of Zurich
S. Lubner*

CYP2D6 selectivity revised: deciphering reaction determinants by well-tempered metadynamics simulations and QM/MM calculations of variants with diverse enzymatic activity. [CC-109]

Charleen Don, University of Basel
M. Smieško*

Evolving a protein scaffold towards catalyzing tetrazol formation using QM/MM simulations and evolutionary computation [CC-110]

Simon Dürr, EPFL Lausanne
N. J. Browning, P. Diamantis, U. Röthlisberger*

Machine Learning Approach with Molecular Dynamics Fingerprints to Predict P-Glycoprotein Substrates and Multidrug Resistance [CC-111]

Carmen Esposito, ETH Zurich
U. E. Lange, A. Stefan, F. Oellien, S. Riniker*

Ab initio free energy computations with machine learning potentials and enhanced sampling [CC-112]

Raimon Fabregat, EPFL Lausanne
A. Fabrizio, B. Meyer, C. Corminboeuf*

Where are our errors in Frozen-Density Embedding Theory coming from? [CC-113]

Mingxue Fu, University of Geneva
C. E. González-Espinoza, A. Zech, N. Ricardi, Y. Gimbal-Zofka, T. Wesolowski*

Computational Screening of Metal-Organic-Frameworks for Applications in Photocatalysis [CC-114]

Maria Fumanal, EPFL Lausanne
G. Capano, K. M. Jablonka, A. Ortega-Guerrero, S. Barthel, B. Smit*, I. Tavernelli*

State specific environment pre-polarisation of environment with point charges within Frozen-Density Embedding Theory [CC-115]

Yann Gimbal-Zofka, University of Geneva
N. Ricardi, A. Zech, T. Wesolowski*

On the accuracy and efficiency of smooth Coulomb potentials [CC-116]

Cristina González-Espinoza, University of Geneva
P. W. Ayers, T. Verstraelen, A. Savin

Gaussian Process-Based Refinement and Assessment of Dispersion Corrections [CC-117]

Stefan Gugler, ETH Zurich
J. Proppe, M. Reiher*

A multiconfigurational analysis of water oxidation catalysis [CC-118]

Ruo Cheng Han, University of Zurich
S. Lubner*

Domain wall-defect interaction in BaTiO₃ by density functional theory [CC-119]

Prateeti Hazarika, University of Bern
U. Aschauer*

Effect of dispersion corrections on ab-initio free energy landscape by machine learning [CC-120]

Theo Jaffrelot Inizan, EPFL Lausanne
R. Fabregat, A. Fabrizio, V. Jurásková, C. Corminboeuf*

Exploiting artificial neural networks in simulation of complex ionic chemical environment [CC-121]

Veronika Jurásková, EPFL Lausanne
K. Rossi, L. Garel, R. Wischert, C. Corminboeuf*, M. Ceriotti*

Evaluating Force Fields Using Cross-Solvation Free Energies [CC-122]

Sadra Kashaf Ol Ghatta, ETH Zurich
P. H. Hünenberger*

A neural network based representation of state-to-state cross sections for atom-diatom collisions [CC-123]

Debasish Koner, University of Basel
O. T. Unke, K. Boe, R. J. Bemish, M. Meuwly*

Alternatives to conventional intermediate states in free energy simulations [CC-124]

Gerhard König, ETH Zurich
S. Riniker*

Solvent scaling in MD simulations [CC-125]

Alžbeta Kubincová, ETH Zurich
P. H. Hünenberger*

Self-ionization of water at aqueous platinum interface [CC-126]

Jinggang Lan, University of Zurich
J. Hutter, M. Iannuzzi*

Charge Transport Behaviors of Oligoacene- and Fused-Thiophene- Based Amorphous Hole Transport Materials [CC-127]

Kun-Han Lin, EPFL Lausanne
C. Corminboeuf*

Enhanced sampling and reweighting methods to understand rare-event kinetics of cyclic peptides [CC-128]Stephanie Linker, ETH Zurich
J. Witek, S. Wang, S. Riniker***Simulating Ion Diffusion in Solid-State Electrolytes using Deep Neural Network Potentials [CC-129]**Aris Marcolongo, IBM Research – Zurich
F. Zipoli, T. Binninger, F. Zipoli, T. Laino***Spectroscopy with RT-TDDFT [CC-130]**Johann Mattiat, University of Zurich
S. Lubert***Non-covalent quantum machine learning corrections to density functionals [CC-131]**Pal Mezei, University of Basel
O. A. von Lilienfeld**Concurrent Optimisation of Organic Donor-Acceptor Pairs through Machine Learning [CC-132]**

Daniele Padula, Empa

Efficient geometric integrators for nonadiabatic quantum dynamics. II. The diabatic representation [CC-134]Julien Roulet, EPFL Lausanne
S. Choi, J. Vanicek***Structural Dynamics of an Excited Donor-Acceptor Complex: Ultrafast Polarized Infrared Spectroscopy and Mixed Quantum/Classical Simulations [CC-135]**Christopher Rumble, University of Geneva
E. Vauthey***Vibrational Spectroscopy of N₃⁻ in the Gas and Condensed Phase. [CC-136]**Seyedeh Salehi, University of Basel
D. Koner, M. Meuwly***Mechanistic Origin of the Diverging Selectivity Patterns in Catalyzed Ethane and Ethene Oxochlorination [CC-137]**Matthias Scharfe, ETH Zurich
G. Zichittella, V. A. Kondratenko, E. Kondratenko, N. López, J. Pérez-Ramírez***Modeling Artificial Water Oxidation – Insights into Reaction Mechanism and Catalyst Design [CC-138]**Mauro Schilling, University of Zurich
S. Lubert***Efficient and Accurate Sampling of Reactive Events [CC-139]**Giovanni Maria Piccini, ETH Zurich
M. Parrinello***Highly efficient Kr/Xe separation from poly(triazine imide) nanopores [CC-140]**Mohammad T. Vahdat, EPFL Lausanne
D. Campi, K. V. Agrawal*, N. Marzari***Machine learning of accurate spin splittings in a large carbene chemical space [CC-141]**Diana Tahchieva, University of Basel
M. Schwilk, A. von Lilienfeld***On water slip confined between two-dimensional materials from *ab initio* molecular dynamics. [CC-142]**Gabriele Tocci, University of Zurich
L. Joly, M. Bilichenko, M. Iannuzzi, J. Hutter***The Effects of S-Nitrosylation on the Conformational Dynamics of Myoglobin [CC-143]**Haydar Turan, University of Basel
M. Meuwly***Exploring the Connections Between Quantum and Semiclassical Instanton Reaction Rate Theories [CC-144]**Christophe Vaillant, EPFL Lausanne
J. O. Richardson, J. Vanicek***Exploring the Chemical Space in the search for improved Azoheteroarene-based photoswitches [CC-145]**Sergi Vela, EPFL Lausanne
C. Krüger, C. Corminboeuf***Electron correlation effects and quantum entanglement measures from multi-configurational wave functions [CC-146]**Vera von Burg, ETH Zurich
J. H. Andersen, M. Reiher***Automated Force-Field Refinement From Experimental Data for Compound Families: Automated Setup of Molecular Topologies [CC-147]**Salomé Walthard, ETH Zurich
M. Pereira Oliveira, P. H. Hünenberger***Error-Propagation by Increments [CC-148]**Thomas Weymuth, ETH Zurich
M. Reiher***Inorganic Chemistry [IC]
Poster Session****Ligand Tuned Multinuclear Copper Complexes as Homogenous Water Oxidation Catalysts [IC-101]**Devi Prasad Adiyeri Saseendran, University of Zurich
G. R. Patzke***Lead-Halide Scalar Couplings in ²⁰⁷Pb NMR of APbX₃ Perovskites (A = Cs, Methylammonium, Formamidinium; X = Cl, Br, I) [IC-102]**Marcel Aebli, ETH Zurich
L. Piveteau, O. Nazarenko, B. M. Benin, F. Krieg, R. Verel*, M. V. Kovalenko***Understanding how ligand substitution influences CO₂ adsorption in a series of sodalite-based MOFs [IC-103]**Mehrdad Asgari, EPFL Lausanne
R. Semino, P. A. Schouwink, I. Kochetygov, O. Trukhina, M. Ceriotti, W. L. Queen***Dinitrogen reduction and N-functionalization by uranium multimetallic complexes [IC-104]**Luciano Barluzzi, EPFL Lausanne
M. Mazzanti*

Towards fast and low-cost synthesis method of Prussian blue and its analogs – cathode materials for Na-ion batteries [IC-105]

Dominika Baster, EPFL Valais Wallis, Sion
W. Oliveira Da Silva, V. Costa Bassetto, H. Girault*

Low-dimensional tin-halides: properties and novel applications [IC-107]

Bogdan Benin, ETH Zurich
S. Yakunin, D. N. Dirin, M. V. Kovalenko*

N₂ coordination in ⁹⁹Tc complexes [IC-108]

Manuel Besmer, University of Zurich
H. Braband, R. Alberto*

Porous networks based on iron(II) clathrochelate complexes [IC-109]

José Bila, EPFL Lausanne
J. Pijeat, F. Fadaei-Tirani, R. Scopelliti, K. Severin*

A multi-application-toolkit: one POM for water splitting, plastic waste recovery and anti-bacteria under light irradiation [IC-110]

Hang Chen, University of Zurich
G. R. Patzke*

Colloidal Routes towards Highly-Monodisperse Intermetallic and Alloyed Nanocrystals [IC-111]

Jasper Clarysse, ETH Zurich
A. Moser, O. Yarema, M. Yarema, V. C. Wood*

Synthesis of two-dimensional zeolitic nanosheets for hydrogen sieving [IC-112]

Mostapha Dakhchoune, EPFL Lausanne
K. V. Agrawal*

Tris-diimine Fe^{II} Spin Crossover Complexes Using Various N-Heterocyclic Ligands [IC-113]

Neel Deorukhkar, University of Geneva
N. Deorukhkar, T. Lathion, C. Besnard, L. Guénée, C. Piguet*

Study of plasmon-enhanced water splitting in a hematite photoanode [IC-114]

Luc Driencourt, University of Basel
B. Gallinet, S. Fricke, C. E. Housecroft, E. C. Constable*

Silicon Oxycarbide – Tin Nanocomposite as a High-Power-Density Anode for Li-Ion Batteries [IC-115]

Romain Dubey, ETH Zurich
P. Vallachira Warriam Sasikumar, F. Krumeich, G. Blugan, K. V. Kravchyk, T. Graule*, M. V. Kovalenko*

Can an Oxidized Zinc Finger Bind Zinc? Reversible Oxidation of Zinc fingers [IC-116]

Moritz Durtschi, University of Zurich
S. Johannsen, R. O. Sigel*

Unprecedented uranium species: from water-stable uranyl(V) to uranium(IV) POM clusters. [IC-117]

Radmila Faizova, EPFL Lausanne
L. Chatelain, R. Scopelliti, F. Fadaei-Tirani, M. Mazzanti*

Re(I) κ^2N -tricarbonyl and κ^3N -dicarbonyl complexes with terpyridine ligands: unusual substituent effects and photocatalytic properties [IC-118]

Ricardo Fernández-Terán, University of Zurich
L. Severy, D. Tilley, P. Hamm, R. J. Fernández-Terán*

Functionalised Boronate Ester-Capped Helicates [IC-119]

Erica Giraldo, EPFL Lausanne
K. Severin*

Oxygen functionalization of carbon molecular sieve membranes to modulate pore-size-distribution for gas separation [IC-120]

Shiqi Huang, EPFL Lausanne
K. V. Agrawal*

Synthesis of nanopores in graphene lattice with a sub-angstrom resolution [IC-121]

Shiqi Huang, EPFL Lausanne
K. V. Agrawal*

N₂P₂ Macrocyclic Iron(II) Catalysts for the Asymmetric Cyclopropanation of Alkenes [IC-122]

Harikrishnan Jayaprakash, ETH Zurich
A. Mezzetti*

DNA-bis(benzene)iron based mechanophores [IC-123]

Emilie Jean-Pierre, University of Fribourg
E. Janett, C. G. Bochet*, K. M. Fromm*

Carbon Dioxide Insertion Reactions Driven by Electron-Rich Uranium(IV) Complexes Supported by Tridentate Non-Innocent Ligands [IC-124]

Nadir Jori, EPFL Lausanne
M. Falcone, R. Scopelliti, M. Mazzanti*

Selective CO₂ capture from Automobile exhausts using polyethylene imine impregnated mesoporous silica. [IC-125]

Anita Justin, EPFL Valais Wallis, Sion
W. L. Queen*

RNA folding of a group II intron investigated by single molecule FRET under various Magnesium(II) concentrations using TIRM and confocal microscopy [IC-126]

Kevin Kraft, University of Zurich
S. Zelger-Paulus, R. Börner, R. O. Sigel*

A comparison of radiolabeling methods for iron oxide nanoparticles [IC-127]

Jennifer Lamb, University of Zurich
J. P. Holland*

Enhancement in liquid-vapor phase transition kinetics of water upon confinement under graphene nanopores [IC-128]

Wan-Chi Lee, EPFL Lausanne
K. V. Agrawal*

Superconductivity in the η -carbide-type oxides Zr₄Rh₂O_x [IC-129]

Keyuan Ma, University of Zurich
J. Lago, F. O. von Rohr*

Tetratopic bis(3,2':6',3'')-terpyridines) and bis(4,2':6',4'')-terpyridines): two different isomers for the synthesis of 3D coordination networks [IC-130]

Giacomo Manfroni, University of Basel

F. Baca, Y. M. Klein, A. Prescimone, E. C. Constable*, C. E. Housecroft*

Silver-Induced Alpha-Helix Formation from Random-Coiled Peptide [IC-131]

Florian Marquet, University of Fribourg

L. Babel, V. Chabert, K. M. Fromm*

Chaperone-mediated crystallization of the early cysteine-labeled protein (Ec-1) [IC-132]

Alejandro Marquez Espinoza, University of Zurich

E. Freisinger*

Ruthenium Complexes with Substituted Pincer-type PYA Ligands for Increased Activity in Transfer Hydrogenation Catalysis [IC-133]

Philipp Melle, University of Bern

J. Thiede, D. Hey, M. Albrecht*

Can high-quality single-layer graphene be really synthesized at low temperature? [IC-134]

Mina Moradi, EPFL Lausanne

M. H. Khan, K. V. Agrawal*

Plant MT3 proteins: The unpredictable MT family [IC-135]

Monica Perinelli, University of Zurich

E. Freisinger*

Installing a metal active centre in peptide scaffolds through an unnatural NHC-amino acid [IC-136]

Matteo Planchestainer, University of Bern

K. Lenzen, F. Paradisi, M. Albrecht*

Precise etching of nanopores in single-layer graphene [IC-137]

Mojtaba Rezaei, EPFL Lausanne

K. V. Agrawal*

2,2'-Bipyridine Ligands in Copper(I)-based dyes for Dye-sensitized Solar Cells: Does a spacer make it better? [IC-138]

Guglielmo Risi, University of Basel

C. E. Housecroft*, E. C. Constable*

Ditopic 3,2':6',3'')-terpyridine ligands: Diversity of coordination assemblies. [IC-139]

Dalila Rocco, University of Basel

A. Prescimone, C. E. Housecroft*, E. C. Constable*

A simple cerium-based fluorescent indicator displacement assay for the selective naked-eye detection of phosphate ions in water [IC-140]

Thibaud Rossel, Gymnase français de Bienne

M. Creus, Students GF Bienne, T. Rossel*

Photoinduced Hydrogen Atom Transfer Reactions Catalyzed by Iridium Hydrides [IC-141]

Mirjam Schreier, University of Basel

X. Guo, J. A. Kübler, O. S. Wenger*

Bioinspired Metal-Complexes as Chelators of Bacterial Metallo- β -Lactamase Zinc Ions [IC-142]

Justine Schwarte, University of Fribourg

K. M. Fromm*

Imidazolylidene copper(II) complexes: synthesis and re-arrangement behaviour [IC-143]

Nathalie Ségau, University of Bern

J. McMaster, G. van Koten, M. Albrecht*

How to Crystallize Coordination Complexes, which are Stable in Water? [IC-144]

Bernhard Spingler, University of Zurich

R. Alvarez

Solution-Phase Deposited Tin Sulfide (SnS) Thin Films For Water Splitting [IC-145]

Jihye Suh, University of Zurich

D. Tilley*

Design of Porous MOF/Polymer Composites for Selective and Enhanced Chemical Separations in Aqueous Media [IC-146]

Daniel Sun, EPFL Valais Wallis, Sion

W. L. Queen*

Self-Assembly of d-f heteronuclear triple helices [IC-147]

Ines Taarit, University of Geneva

S. Guerra, B. Doistau*, C. Piguet*

Cooperativity in Spin Crossover Systems. An Atomistic Perspective on the Devils Staircase [IC-148]

Sergi Vela, EPFL Lausanne

H. Paulsen, S. Vela*

Base Metal Complexes of Chelating Pyridylidene Amide (PYA) Ligands for Oxidation Catalysis [IC-149]

Dide Verhoeven, University of Bern

M. Albrecht*

Single-layer poly(triazine imide) nanosheets for gas sieving [IC-150]

Luis Villalobos, EPFL Lausanne

K. V. Agrawal*

Structure-Property Relations in the $\text{Ca}_{1-x}\text{Sr}_x\text{AlSi}$ Solid Solution [IC-151]

Dorota Walicka, University of Zurich

J. Lago, F. O. von Rohr*

Heteroallenes reduction by dinuclear Yb(II) and Sm(II) complexes supported by siloxide ligands [IC-152]

Aurélien Willauer, EPFL Lausanne

D. Toniolo, R. Scopelliti, F. Fadaei-Tirani, M. Mazzanti*

Self-supported formation of Co-Fe-S box-like structure as a robust bifunctional electrocatalyst [IC-153]

Yong Zhao, University of Zurich

G. R. Patzke*

Medicinal Chemistry & Chemical Biology [MC] Poster Session**Molecular level monitoring of long non-coding RNA self-splicing by means of smFRET [MC-101]**

Esra Ahunbay, University of Zurich

S. Zelger-Paulus, R. Börner, R. K.O. Sigel*

Looking at the biosynthetic pathway of the molybdenum co-factor in search of the missing metabolite for the Moco riboswitch [MC-102]

Fabio Amadei, University of Zurich
S. Gallo, K. Schrader, G. Schwarz, R. K. O. Sigel*

Chemical Approaches to Monitor Collagen Cross-linking in the Extracellular Matrix [MC-103]

Matthew Aronoff, ETH Zurich
N. B. Hentzen, L. Pompizi, S. Kang, H. Wennemers*

Influence of peptide composition for the stability of their Ag(I) complexes [MC-104]

Lucille Babel, University of Fribourg
M. Hologne, O. Walker, K. M. Fromm*

X-ray structure of a second generation peptide dendrimer as Lectin complex at 1.4 Å resolution [MC-105]

Stéphane Baeriswyl, University of Bern
A. Stocker, S. Javor, T. Darbre, J.-L. Reymond*

Factors in bacterial ergothioneine degradation [MC-106]

Mariia Beliaeva, University of Basel
A. R. Stampfli, A. Maurer, F. Leisinger, F. P. Seebeck*

Total synthesis of a species-specific anthranilic acid ascaroside from the nematode *Caenorhabditis nigoni* [MC-107]

Célia Bergame, University of Neuchatel
C. Dong, S. H. von Reuss*

Precision Drugs: A Covalent Strategy to Minimize Side Effects of PI3K Inhibitor Cancer Therapy [MC-108]

Chiara Borsari, University of Basel
E. Keles, I. Buslov, D. Rageot, M. P. Wyman*

Synthetic Accessibility and Natural Product Likeness of GDB Molecules [MC-109]

Sven Bühlmann, University of Bern
J.-L. Reymond*

Luminescent glycoclusters: towards lectin detection as a diagnostic strategy [MC-110]

Joseph Byrne, National University of Ireland Galway

A Genetic Algorithm to Explore the Peptide Chemical Space [MC-111]

Alice Capecchi, University of Bern
J.-L. Reymond*

Design and synthesis of PROTACs HIF-1 α and -2 α degraders [MC-112]

Carlotta Cecchini, University of Geneva
C. Terenzi, V. Ceserani, J. Theurillat, S. Tardy, L. Scapoza*

Luciferase-induced photouncaging: Bioluminescence [MC-113]

Dalu Chang, University of Geneva
N. Winssinger*

Exploring DCAF15 for reprogrammable targeted protein degradation [MC-114]

Seemon Coomar, University of Basel
D. Gillingham*

Radiolabelled ⁶⁸Ga-rotaxanes as non-covalent platforms for supramolecular drug delivery [MC-116]

Faustine d'Orchymont, University of Zurich
J. P. Holland*

Targeted lung cancer bioimaging using multifunctional harmonic nanoparticles [MC-117]

Raphaël de Matos, EPFL Lausanne
J. Vuilleumier, S. Passemard, D. Staedler, S. Constant, L. Bonacina, S. Gerber-Lemaire*

Synthesis and Photophysical Properties of BODIPY-Tethered Trithiolato-Bridged Dinuclear Ruthenium(II)-Arene Compounds [MC-118]

Oksana Desiatkina, University of Bern
E. Păunescu, J. Furrer*

Single-Molecule Imaging of Lipid Droplets with Environment-Sensitive Photoactivatable Probes [MC-119]

Adam Eordogh, ETH Zurich
C. Paganini, D. Pinotsi, P. Arosio, P. Rivera-Fuentes*

Sortase mediated conjugation of triglycine functionalised chelates to Her2 targeting DARPins [MC-120]

Rachael Fay, University of Zurich
J. Schaefer, B. Dreier, A. Plückthun, J. P. Lamb*

A novel Post-Treatment process of medical and pharmaceutical material using scCO₂ [MC-121]

Marco Furlan, eCO2
P. Widmer*

Killing mechanism of antimicrobial peptide dendrimer G3KL investigated by fluorescence microscopy [MC-122]

Bee Ha Gan, University of Bern
T. Darbre, J.-L. Reymond*

Carboxymethylated and methylated DNA damage as a basis for prediction of colon cancer risk [MC-123]

Susanne Geisen, ETH Zurich
T. Kostka, M. T. Empl, P. Steinberg, S. J. Sturla*

Developing the production of radiolanthanide ¹⁶¹Tb and its characterization towards clinical application [MC-124]

Pascal Grundler, Paul Scherrer Institute, Villigen
N. Gracheva, Z. Talip, J. R. Zeevaart, U. Köster, C. Bailat, Y. Nedjadi, T. Duran, R. Schibli, C. Müller*, N. P. van der Meulen*

Structure-activity studies on the photoradiosynthesis of ⁸⁹Zr-DFO-labelled MetMAb for molecular imaging of gastric cancer [MC-125]

Melanie Gut, University of Zurich
S. Klingler, R. Fay, L. Eichenberger, J. P. Holland*

Development of a therapeutic collectin-11 inhibitor to minimize ischemia reperfusion injuries [MC-127]

Rachel Hevey, University of Basel
D. Berta, M. Maraj Martinez, T. Wichers, T. Brunner, M. Smieško, S. Rabbani, D. Ricklin*

Robust DNA Circuit for the Release of Functional Molecular Outputs [MC-128]

Ki Kim, University of Geneva
S. Angerani, D. Chang, N. Winssinger*

Simultaneous photochemical conjugation and ⁸⁹Zr-radiolabelling of antibodies for immuno-PET [MC-129]

Simon Klingler, University of Zurich
L. Eichenberger, J. P. Holland*

Exploring the nature of UV induced RNA-protein cross-linking with the help of CLIR-MS [MC-130]

Anna Knörlein, ETH Zurich
C. Sarnowski, T. de Vries, M. Götze, F. Allain, R. Aebersold, J. Hall*

Structure-activity study and molecular insights in the mode of action of complement C3 inhibitor Cp40 [MC-131]

Christina Lamers, University of Basel
B. Wagner, P. Gros, J. D. Lambris, D. Ricklin*

Discovery of a New Acetylated Lysine Mimic and Optimization of CBP/P300 Bromodomain Inhibitors [MC-132]

Eleen Laul, University of Zurich
V. Pascanu, M. S. Kirillova, A. Dolbois, P. Sledz, A. Caflisch, C. Nevado*

Cross-linkable polymeric contrast agent for high-resolution imaging of the vascular system with X-ray microCT [MC-133]

Ngoc An Le, University of Zurich
W. Kuo, V. Kurtcuoglu, B. Spingler*

Exploration of chlorin e6 derivatives for photodynamic therapy [MC-134]

Ngoc An Le, University of Zurich
M. Kalt, B. Spingler*

Structural and mechanistic basis for anaerobic ergothioneine biosynthesis [MC-135]

Florian Leisinger, University of Basel
R. Burn, M. Meury, P. Lukat, F. P. Seebeck*

Development of a Multifunctional Cyclopentadienyl based Linker for the Design of Novel Cancer Theranostics [MC-136]

Raphael Lengacher, University of Zurich
R. Alberto*

Synthesis of Fluorescent Tools to Better Understand the Canalicular Lipid Transporter System [MC-137]

Michele Leuenberger, University of Bern
S. Bernhard, P. Grossenbacher, B. Stieger, M. Lochner*

Functionalized Proline-Rich Peptides Bind the Bacterial Second Messenger c-di-GMP [MC-138]

Simon Loosli, ETH Zurich
C. A. Foletti, H. Wennemers*

Improved design of miR-CLIP probes towards elucidation of miRNAs functions [MC-139]

Anna Malinowska, ETH Zurich
Y. Wang, J. Hall*

NMR structure determination of the CPEB3 ribozyme [MC-140]

Irina Markova, University of Zurich
S. Johannsen, R. O. Sigel*

Semisynthetic Approaches for the Modification of the Glycosylated Macrolide Antibiotic Fidaxomicin [MC-141]

Andrea Meier, University of Zurich
R. Berg, C. Gertzen, K. Zerbe, M. Gwerder, D. Schäfle, P. Sander, H. Gohlke, K. Gademann*

Triazole-linked organometallic architectures – Adding diversity to trithiolato-bridged dinuclear ruthenium(II)-arene compounds via CuAAC click chemistry [MC-142]

Martin Mösching, University of Bern
O. Desiatkina, E. Păunescu, J. Furrer*

Induction of Reductive Stress in Mitochondria by Enzymatic Activation of a Trialkylphosphine Probe [MC-143]

Jade Nguyen, ETH Zurich
A. Tirla, P. Rivera-Fuentes*

Synthesis and *in vitro* cell-penetration characterization of PROTAC-based platforms [MC-144]

Sara Pannilunghi, University of Geneva
S. Tardy, A. Gouiller, L. Galibert, T. De Smedt, L. Scapozza*

Dissecting the Role of the CBP Bromodomain in Development and Hematologic Malignancies [MC-145]

Vlad Pascanu, University of Zurich
A. Dolbois, E. Laul, K. Rollins, K. Prummel, C. Mosimann, P. Sledz, A. Caflisch, C. Nevado*

Development of Molecular Tools for the Cellular Study of Adenosine A1 Receptors [MC-146]

Barbara Preti, University of Bern
M. Leuenberger, M. Lochner, B. G. Frenguelli, G. Ladds

The HDV-like family: crystal structure of the CPEB3 ribozyme [MC-147]

Anna Ilaria Przytula-Mally, University of Zurich
S. Johannsen, V. Olieric, E. Freisinger, R. K.O. Sigel*

Tirucallic Acid Derivatives: Determination of their Absolute Configuration by Vibrational Circular Dichroism [MC-148]

Jakob Reinhardt, University of Basel
T. Nilsu, A. M. Klemd, O. Danton, M. Smieško, R. Huber, T. Bürgi, C. Gründemann, M. Hamburger*

“Close to Release”: A Bioorthogonal Uncaging Reaction Based On Ring-Closing Metathesis [MC-149]

Valerio Sabatino, University of Basel
T. Ward*

Diverse effects of halogenated 2-aminoethoxydiphenyl borate derivatives on store-operated calcium entry in breast cancer cells [MC-150]

Achille Schild, University of Bern
R. Bhardwaj, M. Hediger*, M. Lochner*

Exocyclic Metallated Tetrapyrrolineporphyrane as a Potential Photosensitizer for Photodynamic Therapy [MC-151]

Lukas Schneider, University of Zurich
M. Larocca, W. Wu, V. Babu, C. König, S. Ferrari, B. Spingler*

“Doubly Orthogonal” Labelling of Peptides and Proteins [MC-152]

Raphaël Simonet-Davin, EPFL Lausanne
R. Tessier, J. de Ceballos, N. Guidotti, J. Waser*, B. Fierz*

Antimicrobial Peptide Dendrimer Chimera active against Multidrug-resistant Bacteria [MC-153]

Sacha Siriwardena, University of Bern
J. L. Raymond*

Single-Molecule Imaging of Active Mitochondrial Nitroreductases using a Photo-Crosslinking Fluorescent Sensor [MC-154]

Zacharias Thiel, ETH Zurich
P. Rivera-Fuentes*

Synthesis of functionalized probes based on GSK7975A to study SOCE [MC-155]

Dominic Tscherrig, University of Bern
R. Bhardwaj, J. Dernic, M. Hediger*, M. Lochner*

Screening and repositioning the candidate drugs for retinoblastoma [MC-156]

Po-Jen Tseng, EPFL Lausanne
P. J. Dyson*

On the Hunt for the Missing Data: 6-Thia-B-norestrogens as Logic, but Neglected Intermediates between Estrogens and Benzothiophene-type SERMs [MC-157]

Carsten Vock, University of Vienna, Austria

Two-photon triggered photorelease of caged molecular cargos from multifunctional harmonic nanoparticles [MC-158]

Jérémy Vuilleumier, EPFL Lausanne
R. De Matos, G. Gaulier, C. Mas, S. Constant, L. Bonacina, S. Gerber-Lemaire*

Capsule Chemistry at the Touch of a Button. A New Tool for Medicinal Chemistry [MC-159]

Tuo Jiang, Synple Chem AG and ETH Zurich
B. M. Wanner, P. L. Nichols, K. Chen, A. McMillan, S. Bordi, J. W. Bode*

**Organic Chemistry [OC]
Poster Session****Radical cyclizations of α -oxy carbon centered radicals [OC-101]**

Emy André-Joyaux, University of Bern
P. Renaud*

Cp*Rh(III)-catalyzed Cyclopropane Ring Expansion for the Synthesis of Pyrrolidinone [OC-102]

Benoit Audic, EPFL Lausanne
N. Cramer*

One-Pot Alkene Hydroboration/Migratory Suzuki-Miyaura Cross-Coupling [OC-103]

Yann Baumgartner, University of Basel
D. Kato, D. Cavalli, O. Baudoin*

Pancake Bonds in Dimeric Diradicals [OC-104]

Annika Bernhardt, University of Zurich
M. Juriček*

Metastable-state photoacids: comparative study of substituent effects [OC-105]

Cesare Berton, EPFL Lausanne
C. Pezzato*, K. Severin*

Synthesis and reactivity of non-cyclometallated Au(III)-F: mild C(sp²)-C(sp) bond formation [OC-106]

Michal Biedrzycki, University of Zurich
A. Genoux, C. Nevado*

Rh-Catalyzed Synthesis of Indenyl Triazenes [OC-107]

Carl Bormann, EPFL Lausanne
F. G. Perrin, K. Severin*

Singlet or Triplet? That is the Question [OC-108]

Daniel Čavlović, University of Zurich
M. Juriček*

Dynamic-Covalent Benzopolysulfane Networks: A New Concept for Thiol-Mediated Cellular Uptake [OC-109]

Yangyang Cheng, University of Geneva
J. López-Andarias, R. Martinent, Y. Okamoto, T. Ward, N. Sakai, S. Matile*

The Synthesis of Helically Chiral and Donor-Acceptor Carbon Nanohoops [OC-110]

Adriano D'Addio, University of Basel
J. Malinčík, T. Šolomek*

The keteniminium chemistry as an efficient tool for the synthesis of 3-aminoheteroles [OC-111]

Dylan Dagoneau, Syngenta Crop Protection AG
A. Kolleth, A. Lumbroso, P. Quinodoz, G. Tanriver, S. Catak, S. Sulzer-Mossé, A. De Mesmaeker*

Straightforward Synthesis of 3-Aminothiophenes Using Activated Amides [OC-112]

Dylan Dagoneau, Syngenta Crop Protection AG
A. Kolleth, A. Lumbroso, P. Quinodoz, G. Tanriver, S. Catak, S. Sulzer-Mossé, A. De Mesmaeker*

Stereoselective Synthesis of Z-Enamides and Enol Ethers from Hypervalent Iodine Reagents [OC-113]

Nina Declas, EPFL Lausanne
P. Caramenti, R. Tessier, M. D. Wodrich, J. Waser*

Ligand-Controlled Chemodivergent Copper-Catalyzed Borylations of 2-Substituted [3]Dendralenes [OC-114]

Camille Desfeux, University of Geneva
C. Mazet*

Nickel-Catalyzed Enantioselective C-H Functionalizations of Heterocycles Enabled by Bulky N-Heterocyclic Carbene Ligands [OC-115]

Johannes Diesel, EPFL Lausanne
A. M. Finogenova, D. Grosheva, N. Cramer*

A green chemical synthesis of reusable palladium nanoparticles from phytochemical resins. Applications for mild and chemospecific hydrogenations of nitroarenes [OC-116]

Mohamed Enneimy, Université de Haute-Alsace
C. Le Drian, J. Becht*

Direct Access to Chiral Secondary Amides by Copper-Catalyzed Borylative Carboxamidation of Vinylarenes with Isocyanates [OC-117]

Daniele Fiorito, University of Geneva
Y. Liu, C. Besnard, C. Mazet*

An Enantioselective/Diastereoconvergent [Cu/Rh] Catalytic Sequence to Access Polyfunctionalized 7-Membered Rings from 1,3-Dienes [OC-118]

Michele Garbo, University of Geneva
C. Mazet*

Epoxide opening ether cyclization mediated by exotic α -hole interactions [OC-119]

Andrea Gini, University of Geneva
M. Paraja, N. Sakai, S. Matile*

Non-oxidative ring opening of strained rings with gold: a mechanistic study [OC-120]

Jorge González, University of Zurich
F. Verdugo, F. López, J. L. Mascareñas, C. Nevado*

Investigating the Herbicidal Properties of Streptol and its Analogues [OC-121]

Tatyana Grayfer, University of Zurich
A. Georgiou, A. Bailly, J. Michel, S. Sieber, L. Eberl, K. Gademann*

Rh(III)-Catalysed C-H (Hetero)arylation of Pyridones and Quinolines with IndoleBX [OC-122]

Ashis Das, EPFL Lausanne
E. Grenet, P. Caramenti, J. Waser*

Peptide Stapling by the Means of Selective Cysteine Alkynylation Using Hypervalent Iodine Reagents [OC-123]

Elija Grinhagena, EPFL Lausanne
J. de Ceballos, J. Waser*

Scorpion-Like Designer Amines for Efficient and Reversible CO₂-Capture from Gas Mixtures [OC-124]

Jan Hanusch, University of Zurich
I. P. Kerschgens, F. Huber, M. Neuburger, K. Gademann*

Anion- π Catalysis on Epoxide-Opening Cascade [OC-125]

Xiaoyu Hao, University of Geneva
X. Zhang, A. Bornhof, J. López-Andarias, W. Liu, J. Wang, A. Pham, N. Sakai, S. Matile*

Towards an Excited State Hammond Postulate [OC-126]

Freya Harvey, University of Fribourg
C. Bochet*

Visible light mediated enantioselective formation of all-carbon quaternary centers on acyclic systems [OC-127]

Cedric Hervieu, University of Zurich
T. Suarez, M. Müller, E. Merino, C. Nevado*

Synthesis of Chiral and Redox-Active Covalent Organic Cages and Macrocycles [OC-128]

Hsin-Hua Huang, University of Basel
T. Šolomek*

Synthesis and characterization of new oxazolidine derivatives [OC-129]

Maksym Karamash, University of Fribourg
M. Giannantonio, A. Crochet, K. M. Fromm*

Synthesis of the First Persistent Helical Non-Kekulé Triplet Diradical [86]Cethrene [OC-130]

Mohebodín Karbasiyoun, University of Zurich
M. Juriček*

1-Acyl Triazenes: Synthesis and Reactivity [OC-131]

Iris Landman, EPFL Lausanne
K. Severin*

Ring Opening of 1,2-Dithiolane and 1,2-Diselenolane, Consequences for Cellular Uptake and Probing of Thiol-Mediated Uptake into Bacteria [OC-132]

Quentin Laurent, University of Geneva
M. Berthet, S. Barluenga, N. Sakai, N. Winssinger*, S. Matile*

An Eco-friendly Route to Reusable Pd-containing Mesoporous Carbons for Mild and Chemospecific Hydrogenations of Nitroarenes [OC-133]

ClaudeLe Drian, Université de Haute-Alsace
M. Enneimy, C. Matei Ghimbeu, J. Becht*

Copper Catalyzed Chemo-, Regio- and Enantioselective Borylation of 1,3-Diene [OC-134]

Yangbin Liu, University of Geneva
D. Fiorito, C. Mazet*

Anion- π Catalysis on Functional Fullerene Oligomers [OC-135]

Wenxing Liu, University of Geneva
J. Wang, A. Bornhof, X. Zhang, J. López-Andarias, X. Hao, A. Pham, N. Sakai, S. Matile*

Bioinspired Synthesis of Lignans [OC-136]

Roger Marti, HEIA Fribourg
S. Brandao, F. Dardano

Synthesis of Molecular Nanoprisms Based on Perylene-3,4,9,10-dicarboximides [OC-137]

Cristian Martinez, University of Basel
T. Šolomek*

Synthesis of possible protein biomarkers as reference materials for retrospective verification of exposure to Chlorine [OC-138]

Severin Martz, University of Fribourg
C. Bochet*, C. Curty*

Dual-photoredox/Ni catalyzed three-component carbofunctionalizations of alkenes [OC-139]

Rahul Mondal, University of Zurich
A. García-Domínguez, C. Nevado*

Palladium-catalyzed Intermolecular Biaryl Atropenantioselective C-H Functionalization [OC-140]

Qui-Hien Nguyen, EPFL Lausanne
S. Guo, N. Cramer*, O. Baudoin*

Advanced wastewater treatment to abate micropollutants with granular activated carbon (GAC) alone and combined with partial ozonation (O₃/GAC) [OC-141]

Christelle Oltramare, Eawag, Dübendorf
A. Hernandez, S. Mangold, M. Böher*, C. McArdell*

Chiral Cp*Co(CO)I₂ Complexes in Asymmetric C-H Functionalization [OC-142]

Kristers Ozols, EPFL Lausanne
Y. Jang, N. Cramer*

Enantioselective Synthesis of Benzonorcaradienes by Chiral Cyclopentadienyl Ruthenium Catalysis [OC-143]

Sung Park, EPFL Lausanne
S. Wang, N. Cramer*

[8] & [9] Cethrenes: Chiroptical & Magnetic Switches [OC-144]

Tomáš Pastierik, University of Zurich
M. Juriček*

Gold Nanoparticle Dimers *via* Acetylene Homocoupling [OC-145]

E. Peters, University of Basel
M. Mayor*

Scenes of Tension Inside the Cell with Selective Mechanosensitive Fluorescent Probes [OC-146]

Francesca Piazzolla, University of Geneva
N. Sakai, S. Matile*

Copper-Catalyzed Insertion of Diazo Compounds into Vinyl Hypervalent Iodine Reagents to Generate Allylic Esters [OC-147]

Guillaume Pisella, EPFL Lausanne
J. Waser*

Synthesis of benzazepinones *via* intramolecular cyclization involving ketene iminium intermediates [OC-148]

Pierre Quinodoz, Syngenta Crop Protection AG
A. Kolleth, D. Dagoneau, A. Lumbroso, A. De Mesmaecker*

Catalytic Cascade Reactions Inspired by Polyketide Biosynthesis [OC-149]

Felix Raps, University of Basel
V. C. Fäseke, D. Häussinger, C. Sparr*

Pd⁰-Catalysed C(sp³)-H Activation: From Direct to Remote Functionalization for the Construction of Medium-Sized Rings [OC-150]

Ronan Rocaboy, University of Basel
O. Baudoin*

Preparation of Indolenines *via* Nucleophilic Aromatic Substitution [OC-151]

Joel Roesslein, University of Zurich
F. Huber, K. Gademann*

Enantioselective C(sp²)-H arylation for the synthesis of warped molecules [OC-152]

David Savary, University of Basel
O. Baudoin*

Synthesis of Novel 3-Monosubstituted s-Tetrazines and Application in the Labeling of Macromolecules [OC-153]

Simon Schnell, University of Zurich
S. Sieber, A. Panchagnula, K. Gademann*

C γ -Substituents as Tools to Influence the Reactivity of Proline Based Catalysts [OC-154]

Martin Schnurr, ETH Zurich
H. Wennemers*

Synthesis of α -aminoboronic acids and α -tertiary amines from potassium acyltrifluoroborates (KATs) [OC-155]

Anne Schuhmacher, ETH Zurich
T. Shiro, M. K. Jackl, J. W. Bode*

Modular Synthesis of α -Amanitin [OC-156]

Philipp Seeberger, EPFL Lausanne
N. Cramer*

Synthesis of Tetraarylethene and Triazoline AIE Emitters [OC-157]

Abdusalom Suleymanov, EPFL Lausanne
K. Severin*

Atom transfer radical addition of a-boryl carbon centered radicals to alkenes for a new cyclopropanation manifold [OC-158]

Nicholas Tappin, University of Bern
W. Michalska, S. Rohrbach, P. Renaud*

Divergent Total Synthesis of (+)-Epicocin G and (-)-Rostratin A Enabled by Double C(sp³)-H Activation [OC-159]

Pierre Thesmar, University of Basel
O. Baudoin*

Catalysis in the Supramolecular Resorcinarene Capsule [OC-160]

Konrad Tiefenbacher, University of Basel
Q. Zhang, K. Tiefenbacher*

Developing Chiral 1,3,2-Diazaphospholenes for Enantioselective Catalysis [OC-161]

John H. Reed, EPFL Lausanne
P. Donets, S. F. Miaskiewicz, N. Cramer*

The Hemiasterlin / E7974 Couple as Training Set for Organic and Natural Products Chemistry Courses in the Field of Life Sciences [OC-162]

Carsten Vock, University of Vienna / Austria

Electron diffraction: A new tool for the structural chemist [OC-163]

Julian Wennmacher, Paul Scherrer Institute, Villigen
T. Gruene, T. Gruene, J. A. van Bokhoven*

Total Synthesis of Heliolactone [OC-164]

Masahiko Yoshimura, ETH Zurich
M. C. Dieckmann, P. Quinodoz, A. De Mesmaecker*

A Mild Diversification Strategy Providing Direct Access to Nitroalkenes, Nitrohydrins, Isoxazolines and Isoxazoles from an NO₂-Redox Active Scaffold [OC-165]

Kun Zhang, ETH Zurich
B. J. Jelier, A. Passera, G. Jeschke, D. Katayev*

Divergent 1,3-Difunctionalization of Aminocyclopropanes [OC-166]

Ming-Ming Wang, EPFL Lausanne
J. Waser*

Unravelling the conductance path through single-porphyrin junctions [OC-167]

Patrick Zwick, University of Basel
M. E. Abbassi, A. Rates, D. Stefani, A. Prescimone, H. S. van der Zant, M. Mayor*, D. Dulic*

A General Approach Towards Collagen Heterotrimers [OC-126]

Nina Hentzen, ETH Zurich
V. Islami, H. Wennemers*

**Physical Chemistry [PC]
Poster Session**
Effects of pressure and temperature on photophysical properties of Sm²⁺ in BaF₂ crystals [PC-101]

Jafar Afshani, University of Geneva

Chemical shift based NMR crystallography directed by unbiased prior constraints [PC-102]

Martins Balodis, EPFL Lausanne

A. Hofstetter, F. M. Paruzzo, G. Stevanato, A. C. Pinon, C. Widdifield, P. Bygrave, G. M. Day, L. Emsley*

Quantum effects in the electron escape from submicron-sized droplets [PC-103]

Loren Ban, ETH Zurich

T. E. Gartmann, B. L. Yoder, R. Signorell*

NMR Studies of Hierarchical Protein Dynamics [PC-104]

Busi Baptiste, EPFL Lausanne

Y. J. Reddy, A. Hofstetter, H. Oshkinat, N. Salvi, M. Blackledge, L. Emsley*

Magnetic selection of neutral alkali-metal doped clusters [PC-105]

Jonathan Barnes, ETH Zurich

S. Hartweg, A. Luski, M. Beck, B. Yoder, E. Narevicius, R. Signorell*

Protein dynamics by MAS NMR: towards the investigation of posttranslational modifications in tubulin [PC-106]

Andrea Bertarello, EPFL Lausanne

B. Baptiste, E. Ebberink, B. Fierz*, L. Emsley*

Polarimetric angle-resolved second harmonic scattering on colloidal TiO₂ nanoparticles in aqueous environments [PC-107]

Marie Bischoff, EPFL Lausanne

A. Marchioro*, S. Roke*

State-to-State Molecule/Surface Scattering Apparatus Using Bolometric Infrared Laser Tagging Detection [PC-108]

Bo-Jung Chen, EPFL Lausanne

D. Auerbach, R. Beck*

Gas-liquid Scattering Dynamics in Crossed Beams [PC-109]

Bruno Credidio, EPFL Lausanne

A. Osterwalder*

Non-linear effects in CsPbBr₃ perovskite in a strong quantum confinement regime [PC-110]

Brrener Rodrigo De Carvalho Vale, EPFL Lausanne

A. Burgos-Caminal, M. Schiavon, J.-E. Moser*

Mass accommodation coefficient retrieval through single-particle photoacoustic spectroscopy [PC-111]

Matus Diveky, ETH Zurich

S. Roy, R. Signorell*

Calibrating a surface-sensitive molecular ruler with 2D ATR-IR spectroscopy: distance dependence of vibrational energy transfer [PC-112]

Ricardo Fernández-Terán, University of Zurich

P. Hamm*

Probing the charge transfer mechanism in pentamethine cyanine dyes [PC-113]

George Fish, EPFL Lausanne

J.-E. Moser*

Femtosecond broadband fluorescence upconversion spectroscopy to study vibrational energy relaxation dynamics [PC-114]

Ina Fureraj, University of Geneva

E. Vauthey*

Doubly-excited 3pnd Rydberg Series of the Magnesium Atom: Theory and Experiment [PC-115]

Matthieu Génévriez, ETH Zurich

D. Wehrli, F. Merkt*

Semiclassical calculation of the electronic coherences in ultrafast charge migration process [PC-116]

Nikolay Golubev, EPFL Lausanne

T. Begusic, J. Vanicek*

Imaging Chemi-Ionisation Processes [PC-117]

Sean Gordon, EPFL Lausanne

S. Tanteri, A. Osterwalder*

How the methyl group position influences the ultrafast deactivation in aromatic radicals [PC-118]

Patrick Hemberger, Paul Scherrer Institute, Villigen

M. Steglich, G. Knopp, P. Hemberger*, P. Hemberger*

High-Resolution VUV-Laser PFI-ZEKE Photoelectron Spectroscopy of the A⁺ 2Σ⁺ state in N₂O⁺ [PC-119]

Holger Herburger, ETH Zurich

U. Hollenstein, F. Merkt*

Errors in NMR crystallography [PC-120]

Albert Hofstetter, EPFL Lausanne

F. M. Paruzzo, A. Anelli, E. A. Engel, M. Balodis, M. Ceriotti*, L. Emsley*

Adiabatic Ionisation Energy of CO₂ [PC-121]

Urs Hollenstein, ETH Zurich

K. Dulitz, F. Merkt

Precision measurements of the ionization and dissociation energies of molecular hydrogen [PC-122]

Nicolas Hölsch, ETH Zurich

M. Beyer, C. Jungen, F. Merkt*

Merged Molecular Beams to Study Ion-Molecule Reactions at Temperatures down to 300 mK [PC-123]

Katharina Höveler, ETH Zurich

J. Deiglmayr, P. Allmendinger, J. Agner, H. Schmutz, F. Merkt*

Exploring Electron-Nuclear Coupling in Molecules with Multidimensional Electronic Spectroscopy [PC-124]

Rebecca Ingle, EPFL Lausanne

L. Mewes, S. Liu, S. Decurtins, M. Chergui*

Light-induced peptide unbinding in the RNase S complex [PC-125]

Brankica Jankovic, University of Zurich

C. Zanobini, O. Bozovic, P. Hamm*

High-Resolution Spectroscopy of metastable He₂ and He₂⁺ [PC-126]

Paul Jansen, ETH Zurich
L. Semeria, F. Merkt*

High-Resolution Gigahertz and Terahertz Spectroscopy of the Isotopically Chiral Molecule *trans*-2,3-dideutero-oxirane (c-CHD-CHDO) [PC-127]

Karen Keppler, ETH Zurich
Z. Chen, S. Albert, V. Schurig, O. Trapp, M. Quack*

Spin and Excited-State Charge Dynamics in Myoglobin [PC-128]

Dominik Kinschel, EPFL Lausanne
C. Bacellar, O. Cannelli, G. F. Mancini, B. Sorokin, F. Lima, T. Katayama, W. Gawelda, C. Milne, M. Chergui*

Tracing nucleation on a molecular level [PC-129]

Jan Krohn, ETH Zurich
M. Lippe, C. Li, K. Dingilian, B. Wyslouzil*, R. Signorell*

Untying the Physico-Chemical Properties of Quinolinium-Based Molecular Knots and Links [PC-130]

Tatu Kumpulainen, University of Geneva
K. Caprice, A. Aster, F. Cougnon*

Ruthenium-based pyrochlores for oxygen evolution catalysis [PC-131]

Denis Kuznetsov, ETH Zurich
M. Awais Naeem, A. Fedorov*, C. R. Müller*

Extraction of Monomer-Cluster Association Rate Coefficients from Water Nucleation Data Measured at Extreme Supersaturations [PC-132]

Chenxi Li, ETH Zurich
M. Lippe, R. Signorell*

Operando Identification of Active Centers of Nickel Iron Catalysts for Water Splitting and the Role of Iron in the Catalytic Activity [PC-133]

Yunchang Liang, EPFL Lausanne
K. Banjac, F. Cometto, F. Cometto, X. Hu*, M. Lingenfelder*

Ultrafast photoreduction of solvated iron compounds probed by VUV photoelectron spectroscopy [PC-134]

Luca Longetti, EPFL Lausanne
T. R. Barillot, M. Puppini, J. Ojeda, C. Arrell, F. van Mourik, M. Chergui*

Mechanism of universal fluorescence quenching of organic dyes by water [PC-136]

Jimmy Maillard, University of Geneva
K. Klehs, C. Rumble, A. Poblador Bahamonde, M. Heilemann, A. Fürstenberg*

Long-term trapping of Stark-decelerated polar molecules [PC-137]

Christian Mangeng, University of Basel
D. Haas, C. von Planta, T. Kierspel, D. Zhang, S. Willitsch*

Study of the Structural and Luminescent Properties of Inorganic Crystals doped with Rare Earth Elements [PC-138]

Asma Mansouri, University of Geneva
J. Christmann, H. Hagemann*

A set of temperature-controlled sources as biophysical tools for native mass spectrometry [PC-139]

Adrien Marchand, ETH Zurich
R. Zenobi*

Surface Characterization of Colloidal Silica Nanoparticles by Second Harmonic Scattering: Surface Potential and Interfacial Water Order [PC-140]

Arianna Marchioro, EPFL Lausanne
C. Lütgebaucks, M. Bischoff, S. Roke*

Mimicking nacre through magnetically driven self-assembly of colloids [PC-141]

Joelle Medinger, University of Fribourg
M. Lattuada*

The link between energy relaxation and structural dynamics: A refined mechanistic picture of the [Pt(ppy)(μ-Bu₂pz)]₂ photophysics [PC-142]

Lars Mewes, EPFL Lausanne
R. A. Ingle, E. Baranoff, S. Megow, H. Böhnke, F. Temps, M. Chergui*

From Molecular Modulation to Supramolecular Engineering for Hybrid Perovskite Solar Cells [PC-143]

Jovana Milić, EPFL Lausanne
D. J. Kubicki, Y. Li, J. Im, L. Emsley*, M. Grätzel*

Towards parity violation in chiral molecules: High resolution FTIR spectroscopy of 1,3-difluoroallene, anharmonic calculations and ro-vibrational analysis of its CF-symmetrical ν₄ and asymmetrical ν₁₂ stretching bands [PC-144]

Eduard Miloglyadov, ETH Zurich
S. Albert, K. Keppler, M. Gottselig, M. Quack*

Towards Measuring the Parity Violating Energy Difference (Δ_{pyE}) between the Enantiomers of Chiral Molecules: Theory and Spectroscopic Experiment [PC-145]

Eduard Miloglyadov, ETH Zurich
G. Wichmann, K. Keppler, G. Seyfang, M. Quack*

No incorporation of dimethylammonium into the black perovskite phase of CsPbI₃, evidenced by solid-state NMR [PC-146]

Aditya Mishra, EPFL Lausanne
D. J. Kubicki, D. Prochowicz, Z. Wang, A. Hagfeldt, M. Grätzel*, L. Emsley*

Transient Absorption study of dilute small molecule organic solar cells [PC-147]

Gareth Moore, University of Bern
A. Jungbluth, M. Causa*, A. Privitera, I. Ramirez, N. Banerji*, M. Riede*

Capturing the ultrafast evolution of excited state chirality with time-resolved CD in the deep ultraviolet [PC-148]

Malte Oppermann, EPFL Lausanne
F. Zinna, J. Lacour, M. Chergui*

NMR-Based Determination of the 3D Structure of the Ligand-Protein Interaction Site without Protein Resonance Assignment [PC-149]

Julien Orts, ETH Zurich

Catalytic Fast Pyrolysis of Lignin Model Compounds by Detecting Reactive Intermediates [PC-150]

Zeyou Pan, Paul Scherrer Institute, Villigen
A. Puente-Urbina, J. A. van Bokhoven*, P. Hemberger*

Heteronuclear long-range Rydberg molecules bound by electron-atom scattering [PC-151]

Michael Peper, ETH Zurich
F. Merkt, J. Deiglmayr*

Magic Rydberg-Rydberg transitions in electric fields [PC-152]

Michael Peper, ETH Zurich
J. Deiglmayr, C. Sanna, H. B. van Linden van den Heuvell,
F. Merkt*

Supramolecular encapsulation of metastable-state photoacids [PC-153]

Cristian Pezzato, EPFL Lausanne
C. Berton, K. Severin, C. Pezzato*

Underestimated Effect of a Polymer Matrix on the Light Emission of Single CsPbBr₃ Nanocrystals [PC-154]

Gabriele Rainò, ETH Zurich
A. Landuyt, F. Krieg, C. Bernasconi, S. Ochsenein, D. N. Dirin,
M. Bodnarchuk, M. V. Kovalenko*

Determination of Size, Shape, Mass and Concentration of Single Aqueous Supersaturated Aerosol Particles [PC-155]

Oliver Reich, ETH Zurich
K. Esat, G. David, J. Cremer, R. Signorell*

The chemical nature of CO₂ adsorption on zeolites [PC-156]

Przemyslaw Rzepka, ETH Zurich
N. Hedin*

Study on NO+O and N+O₂ collision on 2A', 4A' and 2A'' potential energy surfaces [PC-157]

Juan Carlos San Vicente Veliz, University of Basel
D. Koner*

Manipulating the translational and internal degrees of freedom of hydrogen atoms [PC-158]

Simon Scheidegger, ETH Zurich
P. Jansen, H. Schmutz, J. Agner, F. Merkt*

Investigation of Mirror-Image Breakdown in the Stationary Electronic Spectra of 9,10-Bis(phenylethynyl)anthracene by Ultrafast Broadband Fluorescence [PC-159]

Konstantinos Seintis, University of Geneva
G. Cohen, H. Arrou-Vignod, E. Vauthey*

Comparative studies on LiNi_{0.5}Mn_{0.5-x}Co_xO₂ (0 ≤ x ≤ 0.5) cathode materials for lithium-ion batteries [PC-160]

Rajalakshmi Senthil Arumugam, ETH Zurich
R. Shunmugasundaram, V. C. Wood*

Precision Spectroscopy, Coherent Manipulation and State-to-State Chemistry of Single Molecular Ions [PC-161]

Mudit Sinhal, University of Basel
Z. Meir, K. Najafian, S. Willitsch*

Effect of Ionic Liquids on the Excited-States Dynamics of Malachite Green at Dodecane/Water Interface [PC-162]

Jihad Sissaoui, University of Geneva
E. Vauthey*

Broadband Fluorescence Up-Conversion Spectroscopy: A Powerful Tool to Assess Ultrafast Dynamics of Charge Carriers and Excitons in Lead Trihalide Perovskites [PC-163]

Etienne Socie, EPFL Lausanne
J.-E. Moser*

Kinetics of exon unbinding in group II introns by single-molecule FRET and molecular dynamics [PC-164]

Fabio Steffen, University of Zurich
M. Khier, D. Kowerko, R. Börner*, R. O. Sigel*

Excited-state symmetry breaking in novel pyrrolopyrroles – The effect of the position and the strength of the acceptor group [PC-165]

Zoltán Szakács, University of Geneva
E. Vauthey*

Towards cold dipole-dipole collisions in 3D-printed merged electric guides [PC-166]

Silvia Tanteri, EPFL Lausanne
N. Gkogkoglou, J. Zou, S. D. Gordon, A. Osterwalder*

Site-selective and bond-specific dissociation of methane molecule [PC-167]

Harmina Vejjayan, EPFL Lausanne
A. Gutierrez-Gonzalez, R. Beck*

Plasmon-induced slow Electron Injection of Gold nanoparticles into titanium dioxide [PC-168]

Lijie Wang, EPFL Lausanne
T. Rossi, M. Chergui*

Autoionization rates of core-excited magnesium Rydberg atoms in electric fields using the core fluorescence as a reference [PC-169]

Dominik Wehrli, ETH Zurich
M. Génévriez, F. Merkt*

Towards parity violation and tunneling in chiral molecules: An experiment in the mid-infrared range using a pulsed slit jet expansion [PC-170]

Gunther Wichmann, ETH Zurich
E. Miloglyadov, G. Seyfang, M. Quack*

Transient infrared response of a PDZ2 domain protein upon light induced ligand perturbation [PC-171]

Claudio Zanobini, University of Zurich
O. Bozovic, B. Jankovic, P. Hamm*

Fluorescence-lifetime-limited trapping of Rydberg He atoms on a chip [PC-172]

Matija Zesko, ETH Zurich
V. Zhelyazkova, J. Agner, H. Schmutz, F. Merkt*

Studying ion-molecule reactions at low temperatures with a merged-beam set-up [PC-173]

Valentina Zhelyazkova, ETH Zurich
M. Zesko, J. A. Agner, H. Schmutz, F. Merkt*

Sub-picosecond charge transfer in polymer/non-fullerene heterojunction [PC-174]

Yufei Zhong, University of Bern
M. Causa', N. Banerji*

Nanographene Favors Interactions with the Electron Acceptor Rather Than the Electron Donor in a Planar Fused Push-Pull Conjugate [PC-175]

Ping Zhou, University of Bern

M. Volland, L. Wibmer, S. Decurtins, S. Decurtins, S.-X. L. Liu, D. Guldi, R. Häner*, T. Feurer*

Sub-Kelvin stereodynamics study of the $\text{Ne}(\text{P}_2) + \text{N}_2$ reaction [PC-176]

Junwen Zou, EPFL Lausanne

S. D. Gordon, A. Osterwalder*

**Polymers, Colloids & Interfaces [PI]
Poster Session**

Relayed Dynamic Nuclear Polarization to Image the Morphology of Complex Materials [PI-101]

Pierrick Berruyer, EPFL Lausanne

A. C. Pinon, J. Viger-Gravel, W. Lan, G. L. Drisko, J. S. Luterbacher, M. Bardet, C. Sanchez, L. Emsley*

Supramolecular Self-Assembly and Functionalization of DNA-Modified Vesicles [PI-102]

Nutchä Bürki, University of Bern

S. M. Langenegger, R. Häner*

Pt(0)-containing metallosupramolecular polymers as precursors for nanoparticle composites [PI-103]

Claudio Cappelletti, Adolphe Merkle Institute / University of Fribourg

L. Olacchia, E. Oveisi, S. Schrettli, C. Weder*

Alkali Ion Responsive Microgel Systems [PI-104]

Vittoria Chimisso, University of Basel

C. Fodor, W. Meier*

Copolymers of phenylene methylene units and its derivatives: Photoluminescent, Corrosion-Protective Coating Materials [PI-105]

Marco D'Elia, ETH Zurich

Programmable and Dynamic Assembly of Mobile Micromachines [PI-106]

Ahmet Demiroers, ETH Zurich

Highly Elastic Polyrotaxane Binders for Mechanically Stable Lithium Hosts in Lithium Metal Batteries [PI-107]

Ahmed Elabd, University of Fribourg

A. Coskun*

Spatiotemporal Imaging of Water in Operating Voltage-gated Ion Channels Reveals the Slow Motion of Interfacial Ions [PI-108]

Maksim Eremchev, EPFL Lausanne

O. B. Tarun, A. Radenovic, S. Roke*

Biodegradable and pH-Responsive Nanoparticles from Radical Ring-Opening Polymerization [PI-109]

Jens Gaitzsch, University of Basel

J. Folini, J. C. Anderson, W. Meier, J. Gaitzsch*

Hollow silica cubes with customisable porosity [PI-110]

Samuel Gallagher, Zurich University of Applied Sciences ZHAW

O. Trussardi, D. Brühwiler*

Stable Immobilization of Enzyme-Polymer Conjugates in a Porous Silica Monolith [PI-111]

Nicolas Ghéczy, ETH Zurich

C. Hou, P. Walde*

Supramolecular Thermoplastic Materials Based on Polyethylene [PI-112]

Michael Giffin, EPFL Lausanne

D. Görl, H. Frauenrath*

Reinforced Supramolecular Polymer Networks - From Conceptual Design Towards Materials Standardization [PI-114]

Daniel Görl, EPFL Lausanne

S. Haraguchi, O. Oguzhan, H. Frauenrath

Layer-by-Layer Self-Assembly of Cationic and Anionic Supramolecular Polymers [PI-115]

Jovana Jevric, University of Bern

S. M. Langenegger, R. Häner*

Electro-triggered self-assembly and *in-situ* nanoparticle sensitization of supramolecular metal-polyphenolic nanofilms designed for voltammetric sensing of aluminum in blood serum [PI-116]

Agata Krywko-Cendrowska, CNRS

L. Marot, F. Boulmedais*

Linking kinetics to viscoelasticity in dynamic covalent hydrogels by 2D ^1H NMR [PI-117]

Bruno Marco-Dufort, ETH Zurich

M. W. Tibbitt*

Squaraine-containing phosphodiester-linked polymers: variety of compounds for various applications [PI-118]

Larysa Markova, University of Bern

R. Häner*

Ultralight graphene carbon nanofiber aerogels for combined gas and particle filtration [PI-119]

Nicole Moeschlin, Zurich University of Applied Sciences ZHAW

C. Adlhart*

Synthesis of Chitosan-Based Nanomaterials for Condensation of DNA in Gene Therapy of Liver Diseases [PI-120]

Laura Nicolle, EPFL Lausanne

C. Journot, A. Gheata, P. Detampel, T. Einfalt, H. Grisch, M. Williman, B. Thöny, J. Huwyler, S. Gerber-Lemaire*

Complex Chemical Dynamics for Time-Domain Control of Self-Assembly and Supramolecular Gelation [PI-121]

Guido Panzarasa, ETH Zurich

E. R. Dufresne*

Role and influence of carbohydrates on supramolecular self-assembly [PI-122]

Giovanni Picca, University of Bern

R. Häner, S. M. Langenegger

Water Reduction Catalyst Embedded in a Semi-Conducting Polymer [PI-123]

Franziska Rahn, University of Zurich

B. Probst, R. Alberto*

Label-free and charge-sensitive second-harmonic imaging of giant vesicle hydration [PI-124]

David Roesel, EPFL Lausanne
M. Eremchev, S. Roke*

AIE-Active Supramolecular Assemblies of TPE-DNA Conjugates [PI-125]

Simon Rothenbühler, University of Bern
S. M. Langenegger, R. Häner*

Lipid membrane phase transitions involve structural redistribution of interfacial water [PI-126]

Tereza Schönfeldová, EPFL Lausanne
F. Kovacik, H. I. Okur, O. B. Tarun, C. Lütgebaucks, S. Roke*

Conjugated Co-Polymers Derived from Phenanthrene-9,10-dione and Dibenzo[f,h]quinoxaline [PI-127]

Bassam Alameddine, Gulf University for Science and Technology
N. Baig, S. Shetty, B. Alameddine*

Triptycene-Containing Poly(vinylene sulfone) Derivatives From a Metal-Free Thiol-Yne Click Polymerization Followed by a Mild Oxidation Reaction [PI-128]

Bassam Alameddine, Gulf University for Science and Technology
N. Baig, S. Shetty, F. Al-Sagheer, S. Al-Mousawi, B. Alameddine*

Multicomponent alginate-based hydrogels presenting tunable properties for allo- and xenogeneic cell transplantation [PI-129]

Luca Szabó, EPFL Lausanne
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Mechanically Responsive Polymers Based on Dye Interactions [PI-130]

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Chiral Nanoparticles: The Effect of Tacticity in Amphiphilic AB Diblock Copolymers [PI-131]

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Ag@SiO₂ nanorattles for antimicrobial coatings [PI-132]

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Dissolution Inhibition Effect of Diazonaphthoquinone Photoactive Compounds on Positive Tone Photosensitive Polyimides: A Computational Study [PI-133]

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Tip-enhanced Raman spectroscopy for structural analysis of two-dimensional covalent monolayers synthesized on water and on Au(111) [PI-134]

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