

PROGRAM

Thursday, August 08, 2013

- 13:00 – 16:00 Arrival, Registration and Check-In
15:00 – 16:00 COFFEE, REFRESHMENTS
16:00 – 16:15 **Welcome addresses** (Organizing Committee, GDCh, ACS, RSC)
16:15 – 16:20 **Opening remarks** (Prof. Dr. Hans-Dieter Arndt)
16:20 – 16:55 Introduction of all participants (tour de table)

Session 1: Functional Materials

- 16:55 – 17:00 Overview by chair (Prof. Dr. Sven Schneider)
17:00 – 17:15 Prof. Dr. Bettina V. Lotsch, Max Planck Institute for Solid State Research, Stuttgart / Ludwig-Maximilians-Universität, München
Functional Frameworks: Design Strategies and Applications
17:15 – 17:30 Dr. Delia J. Milliron, The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley
Linking nanocrystals to create mesostructured electrochemical materials
17:30 – 17:45 Prof. Dr. Marcio E. Vidotti, Universidade Federal do Paraná
The use of pBDD as platform for the growth of electrocatalytic Ni(OH)₂ nanoparticles and for the construction of hydrodynamic flow devices
17:45 – 18:00 Prof. Dr. Mircea Dincă, Massachusetts Institute of Technology, Cambridge
Electronic and Photophysical Properties of Microporous Metal-Organic Frameworks
18:00 – 18:15 Prof. Dr. Rachel K. O'Reilly, University of Warwick, Coventry
Responsive and functional polymeric nanostructures
18:15 – 18:30 Prof. Dr. Matt Law, University of California, Irvine
Developing quantum dot solids for thin-film photovoltaics
18:30 – 18:45 Prof. Dr. Fernanda C. Stedile, Universidade Federal do Rio Grande do Sul, Porto Alegre
Where and why water vapor incorporates in SiO₂ films thermally grown on SiC or Si substrates?
18:45 – 19:00 Prof. Dr. Thomas W. Hamann, Michigan State University, East Lansing
Molecular and Material Approaches to Advance Dye-Sensitized Solar Cells
19:00 – 20:00 **Light Reception & Music – Be surprised!**
20:00 **DINNER – Barbecue at Lakeside terrace**

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Friday, August 09, 2013

Session 2: Metal-Centered Catalysis

- 08:25 – 08:30 Overview by chair (Prof. Dr. Rachel O'Reilly)
08:30 – 08:45 Dr. Erwin Reisner, University of Cambridge
Solar Water Splitting with Enzymes and Synthetic Catalysts Integrated in Nanostructured Materials
08:45 – 09:00 Prof. Dr. Yun Huang, University of California, Los Angeles
Decipher the Origin of Molecular Recognition towards Inorganic Surface: the Case of Pt
09:00 – 09:15 Prof. Dr. Pedro H. C. Camargo, Universidade de São Paulo
Metallic Nanomaterials with Controlled Shapes, Compositions and Structures for Sensing and Catalysis Applications
09:15 – 09:30 Prof. Dr. Sven Schneider, Georg-August-Universität Göttingen
Catalysis towards ammonia based energy storage: From hydrogen release to Direct Ammonia Fuel Cells
09:30 – 09:45 Dr. Igor Larrosa, Queen Mary University of London
Au, Ag, and Pd in C-H activation: reactivity and selectivity control
09:45 – 10:00 Dr. Kallol Ray, Humboldt-Universität zu Berlin
Lewis-acid Trapping of an Elusive Copper-Tosylnitrene Intermediate
10:00 – 10:15 Dr. Stephen P. Thomas, University of Edinburgh
Iron-catalysed, Highly Regioselective, Synthesis of α -Aryl Carboxylic Acids from Styrene Derivatives and formations
10:15 – 10:30 Dr. Viktoria H. Gessner, Julius-Maximilians-Universität Würzburg
Carbene Complexes from Lithium Methandiides and Carbenoids
10:30 – 10:55 COFFEE BREAK

Session 3: Chemistry in Silico

- 10:55 – 11:00 Overview by chair (Prof. Dr. Anastassia N. Alexandrova)
11:00 – 11:15 Jun.-Prof. Dr. Johannes Kästner, University of Stuttgart
Atom Tunneling: from Astrochemistry to Enzymes
11:15 – 11:30 Prof. Dr. Thomas F. Miller III, California Institute of Technology, Pasadena
Quantum dynamics from classical trajectories: Direct simulation of charge transfer in enzymes and molecular catalysts

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- 11:30 – 11:45 Dr. Alexandre Tkatchenko, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin
Collective van der Waals Interactions in Molecular Systems
- 11:45 – 12:00 Dr. David R. Glowacki, University of Bristol
Non-Equilibrium dynamics and energy relaxation: from gases to liquids to crowds
- 12:00 – 12:15 Dr. Lasse Jensen, The Pennsylvania State University
Molecular Plasmonics From First-Principles
- 12:15 – 12:30 Prof. Dr. Timo Jacob, Ulm University
Theoretical Modeling of Electrochemical Systems
- 12:30 – 13:55 LUNCH

Session 4: Simulation & Modeling

- 13:55 – 14:00 Overview by chair (Prof. Dr. Timo Jacob)
- 14:00 – 14:15 Dr. Robert Paton, University of Oxford
Computer-aided Discoveries of Organic Structures and Selectivity
- 14:15 – 14:30 Prof. Dr. Anastassia N. Alexandrova, University of California, Los Angeles
Insight into metallo-enzyme evolution through multi-scale dynamics modeling
- 14:30 – 14:45 Jun.-Prof. Dr. Birgit Strodel, Research Centre Jülich / Heinrich Heine University Düsseldorf
Modelling protein aggregation related to Alzheimer's disease

International Outreach Session

- 14:45 – 15:00 Miriam Hippchen, German Academic Exchange Service (DAAD), Bonn
- 15:00 – 15:15 Dr. Gerrit Limberg, Alexander von Humboldt Foundation (AvH), Bonn
- 15:15 – 15:30 Dr. Kathrin Winkler, German Research Foundation (DFG), Bonn
- 15:30 – 16:00 Panel Discussion (Moderation: Prof. Dr. Timo Jacob)
- 16:00 – 16:25 COFFEE BREAK

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Session 5: Synthetic methods development

- 16:25 – 16:30 Overview by chair (Prof. Dr. Daniel B. Werz)
- 16:30 – 16:45 Prof. Dr. Tehshik P. Yoon, University of Wisconsin-Madison
Photocatalysis with Visible Light
- 16:45 – 17:00 Prof. Dr. Diogo S. Lüdtkke, Federal University of Rio Grande do Sul, Porto Alegre
Stereoselective Arylation of Aldehydes Using Arylzinc Reagents
- 17:00 – 17:15 Dr. Ai-Lan Lee, Heriot-Watt University, Edinburgh
Development of Gold- and Palladium-Catalysed Reactions
- 17:15 – 17:30 Dr. Edward Anderson, Chemistry Research Laboratory, Oxford
New Developments in the Synthesis and Reactions of Ynamides
- 17:30 – 17:45 Dr. Christophe Aissa, University of Liverpool
Transition metal-catalysed carbon-carbon bond activation
- 17:45 – 18:00 Prof. Dr. Nuno Maulide, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr
Catalytic Rearrangements as Platforms for Total Synthesis and the Discovery of New Reactivity
- 18:00 – 19:00 **General Poster-Session**
- 19:00 – 21:00 **DINNER**
- 21:00 **AFTER-DINNER LECTURE**
Prof. Dr. Dr. h.c. mult. Helmut Schwarz, President, Alexander von Humboldt Foundation
Overcoming frontiers in science: Messages and recommendations of the Humboldt Foundation

PROGRAM

Saturday, August 10, 2013

Session 6: Synthesis and Biosynthesis

- 08:25 – 08:30 Overview by chair (Dr. Edward Anderson)
- 08:30 – 08:45 Dr. Niklaas J. Buurma, Cardiff University
Directed assembly in complex multicomponent systems through quantitative understanding of coupled interactions
- 08:45 – 09:00 Dr. Stefan M. Huber, Technische Universität München
Halogen-Bonds in Organic Synthesis and Organocatalysis
- 09:00 – 09:15 Dr. Stephen Goldup, Queen Mary University of London
An Efficient Chiral Auxiliary Approach to Mechanically Planar Chiral Rotaxanes
- 09:15 – 09:30 Prof. Dr. Daniel B. Werz, Technische Universität Braunschweig
Domino Reactions Initiated by Donor-Acceptor Cyclopropanes
- 09:30 – 09:45 Prof. Dr. Leandro H. Andrade, University of São Paulo
Enzymatic Reactions: From Enzyme Prospection To Synthetic Applications With Hetero-Compounds
- 09:45 – 10:00 Dr. Tanja Gaich, Leibniz University of Hannover
Oxindoles are easy to COPE with. Mimicking the DMAT-Synthase
- 10:00 – 10:15 Dr. Rebecca J. M. Goss, University of St Andrews
Elucidating and Exploiting Biosynthesis
- 10:15 – 10:30 Dr. Tobias A. M. Gulder, University of Bonn
Exploring and Exploiting Bacterial Biosynthetic Pathways
- 10:30 – 10:55 COFFEE BREAK

Breakout session

- 10:55 – 11:00 Overview by chair (Prof. Dr. Hans-Dieter Arndt)
- 11:00 – 12:00 **Discussions in topic groups**
- 12:00 – 12:30 **Panel discussion**
(Moderation: Prof. Dr. Hans-Dieter Arndt / Dr. Hans-Georg Weinig)
- 12:30 – 13:25 LUNCH

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Saturday, August 10, 2013

Session 7: Natural Products

- 13:25 – 13:30 Overview by chair (Prof. Dr. Hans-Dieter Arndt)
- 13:30 – 13:45 Prof. Dr. Hendrik Luesch, University of Florida, Gainesville
Drug Discovery Inspired by Marine Cyanobacteria: Novel Chemistry and Biology
- 13:45 – 14:00 Dr. Jeroen S. Dickschat, Technische Universität Braunschweig
Terpene Biosynthesis in Bacteria and Fungi
- 14:00 – 14:15 Prof. Dr. Hans-Dieter Arndt, Friedrich-Schiller-University, Jena
Dihydropyridines for intercepting the early secretory pathway
- 14:15 – 14:30 Dr. Markus Nett, Leibniz Institute for Natural Product Research and Infection Biology, Jena
Insights into the Noncanonical Biosynthesis of Micacocidin, a Drug Against Mycoplasma pneumoniae
- 14:30 – 14:45 Dr. Andrew Truman, University of Cambridge
Probing the Biosynthesis of Natural Product Peptides: Discovery of New Biosynthetic Chemistry
- 14:45 – 15:00 Prof. Dr. Helge B. Bode, Goethe-Universität Frankfurt am Main
Photorhabdus and Xenorhabdus small talk: signals, antibiotics, toxins and enzyme inhibitors
- 15:00 – 15:20 BREAK

Excursion

- 15:20 – 15:30 Gathering of all participants
- 15:30 – 16:15 Bus departure to Aschau
- 16:15 – 16:30 Aerial tramway
- 16:30 – 18:30 Recreational time or hike to Kampenwand mountain
- 18:30 – 21:15 Sunset dinner at "Die SonnenAlm"
- 21:30 – 21:45 Aerial tramway
- 22:00 – 22:45 Bus return to Seeon

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Sunday, August 11, 2013

Session 8: Tools in Chemical Biology

- 08:25 – 08:30 Overview by chair (Prof. Dr. Danica Fujimori)
- 08:30 – 08:45 Dr. Manuela Tosin, University of Warwick, Coventry
Synthetic probes for the investigation of polyketide biosynthesis
- 08:45 – 09:00 Prof. Dr. Daniel K. Nomura, University of California, Berkeley
Mapping Dysregulated Metabolic Pathways in Disease Using Functional Proteomic and Metabolomic Platforms
- 09:00 – 09:15 Prof. Dr. Christian P. R. Hackenberger, Leibniz Institut für Molekulare Pharmakologie, Berlin / Humboldt Universität zu Berlin
When Staudinger meets Huisgen – New concepts for the synthesis of functional proteins
- 09:15 – 09:30 Prof. Dr. Peng Wu, Albert Einstein College of Medicine, New York
Metabolic Labeling of Fucosylated Glycoproteins in Bacteroides
- 09:30 – 09:45 Prof. Dr. Neal K. Devaraj, University of California, San Diego
Chemical Biology with Novel Bioorthogonal Reactions
- 09:45 – 10:00 Dr. Glenn A. Burley, University of Strathclyde, Glasgow
Unravelling the alternative RNA splicing labyrinth with chemical biological tools
- 10:00 – 10:15 Dr. Edward A. Lemke, European Molecular Biology Laboratory (EMBL), Heidelberg
Semi-synthetic tools to study protein plasticity from the single molecule level to large assemblies
- 10:15 – 10:30 Dr. Ulrike Eggert, King's College London
A chemical approach to understanding cell division
- 10:30 – 10:55 COFFEE BREAK

Session 9: Methods and Processes in Chemical Biology

- 10:55 – 11:00 Overview by chair (Prof. Dr. Christian Hackenberger)
- 11:00 – 11:15 Dr. Marina K. Kuimova, Imperial College London
Mapping microscopic viscosity using molecular rotors
- 11:15 – 11:30 Prof. Dr. Danica G. Fujimori, University of California, San Francisco
Chemical Biology of Protein and Nucleic Acid Methylation
- 11:30 – 11:45 Dr. Claudia Höbartner, Max Planck Institute for Biophysical Chemistry, Göttingen
Chemistry of functional nucleic acids for RNA ligation and labeling

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- 11:45 – 12:00 Dr. Ali Tavassoli, University of Southampton
Genetic Selection of Cyclic Peptide Inhibitors of Protein-Protein Interactions
- 12:00 – 12:15 Dr. Scott T. Phillips, The Pennsylvania State University
New Strategies in Reagent Design for Point-of-Care Diagnostics
- 12:15 – 12:30 Dr. Christoph Rademacher, Max Planck Institute of Colloids and Interfaces, Potsdam
Modulating carbohydrate binding proteins in immune cell regulation
- 12:30 – 12:45 Prof. Dr. Marcelo S. Castilho, Federal University of Bahia, Salvador
***In silico* and *in vitro* approaches towards the development of lead compounds against neglected diseases**
- 12:45 – 13:00 Prof. Dr. Nathan C. Gianneschi, University of California, San Diego
Enzyme-Directed Assembly of Nanoparticle Theranostics *In Vivo*
- 13:00 – 13:30 **Overall conclusion, feedback, closing remarks**
- 13:30 – 14:15 LUNCH
- 14:15 Departure