

Solvation Chemistry and Reactive Molecules

755. WE-Heraeus-Seminar

17 Sep - 23 Sep 2023

at the Physikzentrum Bad Honnef, Germany

**WILHELM UND ELSE
HERAEUS-STIFTUNG**



Program (CET)

Sunday, 17 September 2023

14:00 – 18:00 **Registration**

Chair

15:45 – 16:00 Wolfram Sander **Opening and Welcome**

16:00 – 16:45 Miguel A.
Garcia-Garibay **Strongly Entangled Radical Pairs in
Molecular Nanocrystals**

16:45 – 17:05 Hot Topic 1
Jan Philipp Wagner **Urea-O-Oxides: Criegee Intermediates
from N-heterocyclic Carbenes**

17:05 – 17:35 *COFFEE BREAK*

Chair

17:35 – 17:55 Hot Topic 2
Artur Mardyukov **Preparation and Exploration of Heavier
Pnictogen Species**

17:55 - 18:40 Karina Morgenstern **A Local View on the Influence of
Solvents on the Reactivity of Surface-
Catalyzed Reactions**

18:40 – 20:00 *DINNER*

Chair

20:00 – 20:45 Guy Bertrand **Undressing Carbon**

20:45 **Networking**

Program (CET)

Monday, 18 September 2023

07:30 *BREAKFAST*

Chair

08:45 – 09:30 Steven Kass **Opposites Attract and the
Development of Charge-Activated
Salts**

09:30 – 10:15 Peter Chen **Heterobimetallic d8-d10 Complexes as
Intermediates, Transition States, and
Transition State Analogs for the
Transmetalation Step in Cross-Coupling
Reactions. Investigations in the Gas
Phase, in Silico, in Solution, and in the
Solid State**

10:15 – 10:45 *COFFEE BREAK*

Chair

10:45 – 11:30 Uta Wille **Phenylalanine Residues are Very
Rapidly Damaged by NO₃• in an
Aqueous Environment**

11:30 – 12:15 Vladimir Popik **Media Effects on Photo-SPAAC
Reaction**

12:15 – 12:35 Martina Havenith **The Cluster of Excellence RESOLV**

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Monday, 18 September 2023

12:35 – 14:30 *LUNCH*

Chair

14:30 – 14:50 Hot Topic 3
Gerhard Schwaab **Unlike Twins: H-Bonding in H₂S dimer, the “Big Brother” of Water Dimer**

14:50 – 15:35 Cláudio Nunes **Quantum Tunneling Reactions: Discoveries on the Slippery PES of Arylnitrenes**

15:35 – 16:05 *COFFEE BREAK*

16:05 – 18:05 **Poster session I**

18:05 – 19:30 *DINNER*

19:30 **Networking**

Program (CET)

Tuesday, 19 September 2023

07:30 *BREAKFAST*

Chair

08:45 – 09:30 Benjamin Schwartz **The Role of the Solvent in Turning Photodissociation into Photoisomerization and in Quantum Decoherence**

09:30 – 10:15 Xijie Wang **Mapping Fundamental Chemical Processes in Gas & Liquid Using MeV Electrons**

10:15 – 10:45 *COFFEE BREAK*

Chair

10:45 – 11:05 Hot Topic 4
Anjali Mahadevan **2-Isocyanophenylthiyl Radical and its Iodine-triggered Radical Cyclization in Solid Argon**

11:05 – 11:25 Hot Topic 5
Jared King **Kinetics of the Triplet Excited State of Photoreactive Nanocrystalline 4,4'-Dimethylbenzophenone: Relative Contributions from Intermolecular H-Atom Transfer and Self-Quenching**

11:25 – 12:10 Stefan Grimme **New 'Low-Cost' Electronic Structure Methods for Large Systems**

12:10 – 12:30 Hot Topic 6
Joel Mieres Perez **Theoretical Study of Carbenes on Metal Surfaces**

Program (CET)

Tuesday, 19 September 2023

12:30 – 14:25 *LUNCH*

Chair

14:25 – 15:10 Peter Schreiner **The Intrinsic Barrier Width and its Role in Chemical Reactivity**

15:10 – 15:55 Götz Bucher **Influence of Solvation on Lifetimes of Reactive Quinoid Molecules and Triplet Excited States: Two Case Studies**

15:55 – 16:30 *COFFEE BREAK*

Chair

16:30 – 17:15 Patrick Nürnberger **A Time-Resolved Look on Photochemical Processes for which Adjacent Molecules Play a Crucial Role**

17:15 – 18:00 Hendrik Zipse **The Stability of O-Centered Radicals**

18:00 – 18:20 Hot Topic 7
Enrique Mendez-Vega **Taming Unstable Carbocations in Gas-Phase and Water Ice Matrices**

18:20 – 19:55 *DINNER*

19:55 **Networking**

Program (CET)

Wednesday, 20 September 2023

07:30 *BREAKFAST*

Chair

08:45 – 09:30 Manabu Abe **Is π -Single Bonding (C– π –C) Possible? A Challenge in Organic Chemistry**

09:30 – 10:15 Igor Alabugin **Energy of Chemical Bonds as a Driving Force for Organic Reactions: Molecular Springs, Stereoelectronic Frustration, and Electron Upconversion**

10:15 – 10:45 *COFFEE BREAK*

Chair

10:45 – 11:30 Viktoria Gessner **Ligand Exchange at Carbon in Metallated Ylides: Synthetic Entry to Elusive Species**

11:30 – 12:15 Burkhard König **Generation of Carbanions by Light**

12:15 – 12:35 Hot Topic 8
Takuya Kodama **Synthesis, Structure, and Reactivity of Tetrylenes Bearing a Phenalenyl-Based Ligand**

12:35 – 14:00 *LUNCH*

14:05 – 14:15 **Conference Photo**
(in the front of the main entrance, before departure to Excursion)

14:15 – 22:15 **Excursion and Dinner**

Program (CET)

Thursday, 21 September 2023

07:30

BREAKFAST

Chair

08:45 – 09:30

Holger Bettinger

Access to and Properties of the Strained Heteroaromatic Benzoborirene Motif

09:30 – 10:15

Fabien Borget

Interstellar Iced Solvation - from Laboratory Studies to a Space Mission Instrument Conception

10:15 – 10:45

COFFEE BREAK

Chair

10:45 – 11:30

Yuan-Pern Lee

Reactive Molecules Investigated with Para-Hydrogen Infrared Matrix Spectroscopy

11:30 – 12:15

Murthy Gudipati

Solvation of Electrons, Ions, and Organics in Astrophysical and Planetary Ices

12:15 – 12:35

Hot Topic 9
André Eckhardt

Spectroscopic Characterization of Interstellar Relevant Imine Species

Program (CET)

Thursday, 21 September 2023

12:35 – 14:30 *LUNCH*

Chair

14:30 – 15:15 Christian Merten **VCD Spectroscopy Under Cryogenic Conditions: Of Matrix Effects and Photochemistry of Chiral Molecules**

15:15 – 16:00 Henrik Ottosson **Excited State Aromaticity and Antiaromaticity: From Scopes to Pitfalls**

16:00 – 16:45 Takashi Kubo **Recent Studies on π -Expanded Trinaphtho[3.3.3]propellane**

16:45 -18:30 **Poster session II**

18:30 - 20:00 *DINNER*

20:00 **Networking**

Program (CET)

Friday, 22 September 2023

07:30 *BREAKFAST*

Chair

08:45 – 09:30 Anna Gudmundsdottir **Turning off and On Photodynamic Behavior of Organic Azide Crystals**

09:30 – 10:15 Gary Douberly **Tba**

10:15 – 10:45 *COFFEE BREAK*

Chair

10:45 – 11:30 Patrick Hemberger **Ketenes in Heterogeneous Catalysis: Blessing or Curse?**

11:30 – 12:15 Udo Brinker **Carbene 1,3-C–H Bond Insertion Reactions: Potential Sources of Cyclopropatetrahedrane**

12:15 – 13:00 Dean Tantillo **Dynamic Effects on Selectivity of Organic Reactions in Solvent**

13:00 – 14:30 *LUNCH*

Chair

14:30 – 15:15 Josef Michl **Porphene and Porphite: Porphyrin Analogs of Graphene and Graphite**

15:15 – 16:00 Dominik Munz **A Plumba Triplet Carbene**

Program (CET)

Friday, 22 September 2023

16:00 – 16:30 *COFFEE BREAK*

Chair

16:30 – 17:15 Rainer Herges **Early Detection of Cancer by Metabolic Imaging**

17:15 – 17:45 Scientific Organizers **Poster Prize Awards & Closing Remarks**

17:45 *HERAEUS DINNER*
(social event with cold & warm buffet and complimentary drinks)

Saturday, 23 September 2023

08:00 *BREAKFAST*

End of the seminar and departure

NO DINNER for participants leaving on Sunday! A self-catering breakfast will be provided on Sunday.