Physical Organic Chemistry:

Recent developments in instrumentation, structure, theory, and mechanisms

PROGRAM

Time	Monday, Feb. 18, 2019
08:00–10:00	*Arrival, Registration, Check-in, Breakfast*
10:30–10:40	Welcome *Peter R. Schreiner and Christina M. Thiele*
	Chair: AnnMarie O'Donoghue
10:40–11:25	The subtle mechanisms of deceptively simple carbonyl hydrosilylations *Martin Oestreich, TU Berlin*
11:25–11:50	Subensemble-Selective Photochemistry by Mixed IR/VIS Two-Dimensional Spectroscopy *Jens Bredenbeck, U Frankfurt*
11:50–12:15	VCD spectroscopy as tool to investigate substrate binding in asymmetric catalysts *Christian Merten, U Bochum*
12:15-12:40	Coulomb Explosion Imaging and Coincidence *Martin Pitzer, Weizmann Institute of Science*
12:45–14:15	**Lunch**
	Chair: Boris Rybtchinski
14:15–15:00	Asymmetric additions to racemates *Stephen Fletcher, U Oxford*
15:00–15:45	IR-induced chemistry: from conformational changes to bond-breaking processes *Rui Fausto, U Coimbra*
15:45–16:15	**Coffee Break**
	Chair: Ryan Gilmour
16:15–17:00	Poster flash talks (10 Posters / 3 min)
	Chair: Dorota Gryko
17:00–17:45	Energy span model: building bridges between computational and experimental catalysis *Sebastian Kozuch, Ben Gurion U Negev*
17:45–18:30	Making Molecules Better *Jonathan Goodman, U Cambridge*
18:45	**Dinner**

Time	Tuesday, Feb. 19, 2019
07:30 – 08:30	**Breakfast**
	Chair: Martin Oestreich
08:30–09:15	Mechanism-based approach to new radical cyclisation cascades *David Procter, U Manchester*
09:15–09:40	Beyond Conventions and Comfort Zones: NHC Stabilized radicals *Julia Rehbein, U Regensburg*
09:40–10:25	Mechanistic understanding of chemoselectivity in NHC and BAC organocatalysis *AnnMarie O'Donoghue, Durham U*
10:25–11:00	**Coffee Break**
	Chair: Ruth Gschwind
11:00–11:25	Aerobic Functionalization of Carbonous π-Bonds by Means of Rationally Designed Selenium-Catalysis *Alexander Breder, U Göttingen*
11:25-11:50	Electrons from functionalized diamond surfaces, a novel tool for photocatalysis *Anke Krüger, U Würzburg*
11:50–12:15	Resolving the Mechanism of Peroxidative Cell Death Using Physical Organic Chemistry *Derek Pratt, U Ottawa*
12:15–12:40	Triplet Phenylphosphinidene: Synthesis, structure, and reactivity *Artur Mardyukov, JLU Giessen*
12:45–14:15	**Lunch**
14:15–16:15	Poster Session and **Coffee Break**
	Chair: Peter Chen
16:15–17:00	Exploiting physical organic principles in reaction design *Ryan Gilmour, U Münster*
17:00-17:25	Conformational Dependence of σ-Delocalization *Josef Michl, U Colorado/Boulder and IOCB, Prague*
17:25–18:10	Dynamic foldamers as biomimetic communication devices *Jonathan Clayden, U Bristol*
18:10–18:25	About the Wilhelm and Else Heraeus Foundation *Stefan Jorda, WE-Heraeus-Stiftung, Hanau*
18:45	**Dinner**

Time	Wednesday, Feb. 20, 2019
07:30 – 08:30	**Breakfast**
	Chair: Stephen Fletcher
08:30–09:15	Intermediates, interactions and transition states in photo- and organocatalysis *Ruth Gschwind, U Regensburg*
09:15–09:40	Mechanistic insight into homogeneous catalysis from multi-nuclear high resolution FlowNMR spectroscopy *Ulrich Hintermaier, U Bath*
09:40–10:05	Structural insights into polymer micelles from solid-state NMR and complementary tools *Ann-Christin Poeppler, U Würzburg*
10:05-10:30	Tuning redox potentials in photocatalysis: Strategies for C O-bond activation and broadly applicable metal-free photoredox catalysts *Kirsten Zeitler, U Leipzig*
10:30–11:00	**Coffee Break**
11:00–11:15	**Conference photo** (in the front of the lecture hall)
	Chair: Oliver Trapp
11:15–11:40	Multicomponent Catalytic Machinery: How the Machine Speed Impacts Catalytic Activity *Michael Schmittel, U Siegen*
11:40–12:05	Transient Intermediates in the Phosphane-Mediated Trimerization of Isocyanates *Hendrik Zipse, LMU Munich*
12:05–12:30	On the Mechanism of organocatalytic glycosylations *Eoghan McGarrigle, University College Dublin*
12:30–14:15	**Lunch**
14:15–16:15	Poster Session and **Coffee Break**
	Chair: Jonathan Clayden
16:15–17:00	Early pathways to life: Mechanisms to molecular evolution and homochirality *Oliver Trapp, LMU Munich*
17:00–17:25	Memory of Chirality in Flow Electrochemistry *Thomas Wirth, U Cardiff*
17:25–18:10	Elucidating crystallization mechanisms by cryogenic electron microscopy *Boris Rybtchinski, Weizmann Institute of Science*
18:45	**HERAEUS DINNER** *(social event with cold & warm buffet with complimentary drinks)*

Time	Thursday, Feb. 21, 2019
07:30 – 08:30	**Breakfast**
	Chair: Jonathan Goodman
08:30–09:15	Quantifying dispersion effects on structure and bond strengths in the gas phase and in solution *Peter Chen, ETH Zurich*
09:15–09:40	Reversible Hydrogen Activation by a Pyridonate Borane Complex: Combining Frustrated Lewis Pair Reactivity with Boron-Ligand Cooperation *Urs Gellrich, JLU Giessen*
09:40–10:25	Photoinduced porphyrinoid catalysis - the need to elucidate the mechanism *Dorota Gryko, Polish Academy of Sciences*
10:25–11:00	**Coffee Break**
	Chair: David Procter
11:00–11:45	Deciphering the structure, dynamics, and chirality of complex molecules *Melanie Schnell, DESY*
11:45–12:30	Electrostatic Gating and Solvent Holes in the Mechanism of Carbocation Reactions *Daniel Singleton, Texas A & M U*
12:30–12:45	Closing remarks *Christina M. Thiele and Peter R. Schreiner*
12:45–14:15	**Lunch**
14:15	**Departure**