

**Photoinduced, Charge-Driven,  
and Molecular Processes  
under Confinement**

**796. WE-Heraeus-Seminar**

**24 – 28 September 2023**

**at the Physikzentrum Bad Honnef, Germany**

**WILHELM UND ELSE  
HERAEUS-STIFTUNG**



# Program

**Sunday, 24 September 2023**

16:00 – 21:00	Registration	
17:20 – 17:30	Karina Morgenstern	<b>Opening remarks</b>
17:30 – 18:30	Miquel Salmeron	<b>Structure and reactions at solid-liquid interfaces</b>
18:30	<i>BUFFET SUPPER</i>	
19:30 – 20:30	Christiane Ziegler	<b>Metallacrowns on Surfaces – how a multi-method approach reveals the details</b>

# Program

Monday, 25 September 2023

08:00	<i>BREAKFAST</i>	
09:00 – 10:00	Kristina Tschulik	<b>Utilizing single entity and spectro-electrochemistry to better understand electrocatalysis in confinement</b>
10:00 – 11:00	Yi-Lun Ying	<b>Looking at single-molecule reaction through a nanopore</b>
11:00 – 11:30	<i>COFFEE BREAK</i>	
11:30 – 12:30	André Laschewsky	<b>Polymer self-assembly driven by charge- or photo-induced processes, versus charge- or photo-induced processes driven by polymer self-assembly: Chicken or the egg?</b>
12:30 – 12:45	Lidón Pruñonosa Lara	<b>Controlled light induced switching of Co(II) coordination cage structures</b>
12:45 – 13:00	Alexandre Walther	<b>Guest-induced transformation and chiral self-discrimination in azulene-based coordination cages</b>
13:00 – 13:10	<b>Conference Photo</b> (in the front of the lecture hall)	
13:10	<i>LUNCH</i>	

# Program

Monday, 25 September 2023

14:30 – 14:45	Julien Rowen	<b>Heavy-atom tunneling in the ring expansion of fluorenylazirines</b>
14:45 – 15:00	Chao-Nan Yang	<b>Observing confined local oxygen-induced reversible thiol/disulfide cycle with a protein nanopore</b>
15:00 – 16:00	Larissa von Krbek	<b>Stimuli responsiveness in molecules, cages, and dynamic libraries</b>
16:00 – 16:30	<i>COFFEE BREAK</i>	
16:30 – 17:30	<b>Flash talks I</b>	
	Iheb Baklouti Nicola Bogó Yuyin Du Kseniya Gorbatenko Guillaume Hoffmann Lea Klausfering Samantha Muhring-Salamone Maximilian Notheis David Ocklenburg Boutaina Rezki Philip Schreyer Marius Spallek Lion Luca Stiewe Gers Tusha Ertugrul Yalcin	
17:30	<i>DINNER</i>	
18:30	<b>Poster session I</b>	

# Program

**Tuesday, 26 September 2023**

08:00	<i>BREAKFAST</i>	
09:00 – 10:00	Amar Flood	<b>Confining anions inside cyanostar macrocycles to stabilize, modify and amplify their reactivity</b>
10:00 – 11:00	Gonzalo Abellan	<b>Carbon nano-onions: Potassium intercalation and reductive covalent functionalization</b>
11:00 – 11:30	<i>COFFEE BREAK</i>	
11:30 – 12:30	Angelika Kühnle	<b>Hydration layers at surfaces: Attraction or confinement?</b>
12:30 – 12:45	Michael Buchmeiser	<b>Olefin metathesis under confinement in mesoporous supports</b>
12:45 – 13:00	Lucy Zhao	<b>Functional template for light-controlled charge regulation in confined mesopores</b>
13:00	<i>LUNCH</i>	
14:30 – 14:45	Florian Albrecht	<b>Selectivity in single-molecule reactions by tip-induced redox chemistry</b>
14:45 – 15:00	Aisha Ahsan	<b>Kinetically induced phase transitions for discrete numbers (<math>1 \leq n \leq 12</math>) of atoms inside quantum confinements</b>
15:00 – 19:00	<b>Excursion</b>	
19:00	<i>HERAEUS DINNER</i> (social event with cold & warm buffet with complimentary drinks)	

# Program

Wednesday, 27 September 2023

08:00	<i>BREAKFAST</i>	
09:00 – 10:00	Gregori Ujaque	<b>Modelling reactivity in the confined space of metallocages</b>
10:00 – 11:00	Rafal Klajn	<b>Supramolecular machinery for disequilibrating azoarenes</b>
11:00 – 11:30	<i>COFFEE BREAK</i>	
11:30 – 12:30	Gerhard Klebe	<b>Drug-target mode-of-action analysis: A case of confinement-controlled chemistry?</b>
12:30 – 12:45	Johanna Angona	<b>Characterization and dealloying of single micelle-nucleated agau nanoparticles by scanning electrochemical cell microscopy</b>
12:45 – 13:00	Fan Gao	<b>Identification of chiral amino acids in a single peptide using an electrostatically asymmetric nanopore</b>
13:00	<i>LUNCH</i>	

# Program

Wednesday, 27 September 2023

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|---------------|--|---|
| 14:30 – 14:45 | Robert Lehn  | <b>Automated local polymer writing into a mesoporous silica thin film using a commercially available fluorescence microscope and oxygen tolerant PET-RAFT</b> |
| 14:45 – 15:00 | Elie Benchimol   | <b>Controlling self-sorting: stimuli responsive multi-cage systems</b>  |
| 15:00 – 16:00 | Marie-Laure Bocquet  | <b>Reactive liquid water with 2D materials from AIMD: water as a ion reservoir , a collective hydron and a molecular ligand</b>                               |
| 16:00 – 16:30 | <i>COFFEE BREAK</i>  |   |
| 16:30 – 17:30 | <b>Flash talks II</b>  |   |
|               | Mercè Alemany-Chavarria<br>Dave Austin<br>Frederike Beyer<br>Adrian Buchmann<br>Sebastian Hütgens<br>Malavika Kalarikkal<br>Clemens Müller<br>Lilian Najm Alsaye<br>Melinda Nolten<br>Yong-He Pan<br>Simon Christian Rickert<br>Lisa Schardt<br>Dipesh Somvanshi<br>Rinshad VA<br>Houyang Xu |   |
| 17:30         | <i>DINNER</i>  |   |
| 18:30         | <b>Poster session II</b>   |   |

# Program

Thursday, 28 September 2023

08:00	<i>BREAKFAST</i>	
09:00 – 10:00	Miguel A. Garcia-Garibay	<b>Triplet quantum chain reactions in crystalline dewar benzenes</b>
10:00 – 11:00	Yoko Sakata	<b>Development of kinetically-controlled molecular recognition systems</b>
11:00 – 11:30	<i>COFFEE BREAK</i>	
11:30 – 12:30	Talat Rahman	<b>Confinement-induced enhanced reactivity of single atom catalysts: theory meets experiments</b>
12:30 – 13:00	Karina Morgenstern	<b>Closing remarks</b>
13:00	<i>LUNCH</i>	

**End of the seminar and departure**

*NO DINNER for participants leaving on Friday; however, a self-service breakfast will be provided on Friday morning*