



865. WE-Heraeus-Seminar

Confinement Control on the Molecular Level: Principles, Mechanisms, Applications

13 Sep – 17 Sep 2026
at Physikzentrum Bad Honnef

Geometrical confinement is relevant to various disciplines, ranging from the natural sciences via the life sciences to the material science field. Confinement effects have far-reaching influences. They shape efficient hydrodynamic flows, deepen the understanding of biological processes, advance carbon capture technologies, and provide new chemical reactivities. So far, much of the research has focused on demonstrating the importance of confinement in physical and chemical systems while neglecting the fundamental principles that govern these effects. Thus, not much is known about how and why exactly confinement effects modulate key physical phenomena, alter reactivities, or change product selectivity and material properties. As a result, essential questions remain unanswered — what are the underlying physical mechanisms at play in confinement, and how do they alter atomic interactions and influence dynamical properties?

Whereas selected specific cases and systems have been studied by experimental computational means, the prediction of confinement effects remains challenging due to a lack of general rules and a common language. With the help of the WE-Heraeus foundation, we will bring together experimentalists and theoreticians to discuss recent findings, match these with confinement effects in 2D, 1D, or 0D spaces, and develop general guidelines that will be applied in calculations and machine learning. In the interdisciplinary WE-Heraeus seminar, we will connect early career researchers with established scientists to create solid scientific networks.

Detailed Scientific Programme

Sunday, 13.09.2026		
		Arrival and Check-in
	15:30 – 16:30	Welcome Coffee Break
Session 1 <i>Chair: Karina Morgenstern</i>	16:30 – 17:00	Opening Remarks – Organizers
	17:00 – 18:00	Jennifer MacLeod <i>Confinement as a Design Principle in Surface Nanoscience</i>
	18:00 – 19:00	Buffet Supper
Session 2 <i>Chair: Karina Morgenstern</i>	19:00 – 20:00	Niels Hansen <i>Leveraging classical density functional theory and molecular simulations to elucidate confinement effects in micro- and mesoporous materials</i>

Monday, 14.09.2026		
	08:00 – 09:00	Breakfast
Session 3 Chair: Poul Petersen	09:00 – 10:00	Paul Lusby <i>Bio-inspired Cage Catalysis</i>
	10:00 – 11:00	Gregori Ujaque <i>From Encapsulation to Catalysis in Nanocages</i>
	11:00 – 11:30	Coffee Break
Session 4 Chair: Lars Schäfer	11:30 – 12:30	Joost Reek <i>Catalyst encapsulation strategies and the effects of confinement on catalytic events</i>
	12:30 – 12:45	Irina Cuesta <i>Computational Insights into Diels–Alder Rate Acceleration inside $[Pd_6L_4]^{12+}$ Coordination Cages</i>
	12:45 – 13:00	Lucas Araujo <i>Confinement-Controlled Macrocyclic Urea Formation</i>
	13:00 – 14:30	Lunch
Session 5 Chair: Axel Rosenhahn	14:30 – 15:30	Hannah Kurz <i>Novel Design Strategies for Multifunctional Coordination Cages</i>
	15:30 – 15:45	Kai Zhang <i>Confined water affects mechanical properties of hydroplastic materials</i>
	15:45 – 16:00	Maya Heine <i>Trapped electron induced photodesorption</i>
	16:00 – 16:30	Coffee Break
Session 6 Chair: David van Craen	16:30 – 16:45	Laurie Stevens <i>Bridging Accuracy and Sampling: Insights into dAMP Solvation from ML-potentials</i>
	16:45 – 17:00	Russell Kajouri <i>Employing Extended Langmuir Adsorption Model for Predicting Gas Uptake in Liquid-Filled Slit Pores</i>
	17:00 – 18:00	Flash Talks I (Posters 01 to 11)
	18:00 – 19:00	Dinner
	19:00 – 22:00	Poster Session I (Posters 01 to 11)

Tuesday, 15.09.2026		
	08:00 – 09:00	Breakfast
Session 7 Chair: Axel Rosenhahn	09:00 – 10:00	Marie-Pierre Gageot <i>Water at aqueous oxide interfaces: their modeling by DFT-MD, wettability, spectroscopy</i>
	10:00 – 11:00	Shadi Fatayer <i>Generating monolayer amorphous carbon by on-surface synthesis</i>
	11:00 – 11:30	Coffee Break
Session 8 Chair: Karina Morgenstern	11:30 – 12:30	Katrin Domke <i>Raman Views of Molecular Confinement: From Nafion Pores to Plasmonic Gaps</i>
	12:30 – 12:45	Bashar Moussa <i>Solvation shell spectroscopy of supported lipid bilayers</i>
	12:45 – 13:00	WE-Heraeus Foundation
	13:00 – 14:30	Lunch
Session 9 Chair: Lars Schäfer	14:30 – 14:45	Antonio J. Martínez-Martínez <i>Adaptive Main-Group Metal Coordination Cages: Reversible Assembly and Guest Recognition in Water</i>
	14:45 – 15:00	Aleksandr Mikhherdov <i>Multi-stimuli Transformations of Pd(II) Supramolecular Assemblies</i>
	15:00 – 19:00	Excursion: hiking to Drachenfels and Schloss Drachenburg Possible to stop in a Café on the way, and/or visit the Schloss Drachenburg
	19:00 – 22:00	Heraeus Dinner (social event with cold & warm buffet and complimentary drinks)

Wednesday, 16.09.2026

	08:00 – 09:00	Breakfast
Session 10 <i>Chair: Hannah Kurz</i>	09:00 – 10:00	Cheng-Yong Su <i>The cage-confined photocatalysis by using MOCs as supramolecular reactors</i>
	10:00 – 11:00	Venkat Kapil <i>Machine learning-based first-principles simulations of nanoconfined water</i>
	11:00 – 11:30	Coffee Break
Session 11 <i>Chair: Guido Clever</i>	11:30 – 12:30	Ebba Matic <i>Host-guest chemistry in systems and catalysis</i>
	12:30 – 12:45	Luca Marie Sicking <i>Electrochemical Investigation of Hydrogen Transport in Anodized Aluminium Oxide Nanochannels</i>
	12:45 – 13:00	Mandy Hoffmann <i>Electrified Graphene-Interfaces as a Model for Nanoconfined Electrolytes: A Self-Consistent Machine-Learned Approach</i>
	13:00 – 13:10	Conference Photo (in front of the lecture hall)
	13:10 – 14:30	Lunch
Session 12 <i>Chair: Poul Petersen</i>	14:30 – 15:30	Sofia Kolin <i>Different pores, different dynamics: How confinement shapes molecular transport</i>
	15:30 – 15:45	Qixuan Li <i>Role of acids in stabilizing Reverse Micelles: the case of Dodecyl Sulfate</i>
	15:45 – 16:00	Johannes Fiedler <i>Rethinking molecular interactions under confinement: an open quantum system perspective</i>
	16:00 – 16:30	Coffee Break
Session 13 <i>Chair: Christian Merten</i>	16:30 – 16:45	Malte Feßner <i>Site-effects in matrix isolation investigated with multidimensional IR spectroscopy</i>
	16:45 – 17:00	Mingkai Zhao <i>Acceleration of Azide-Alkyne Cycloaddition reactions in Octa-amino Bis-calix[4]pyrrole Cages in Organic/Aqueous Solution</i>
	17:00 – 18:00	Flash Talks II (Posters 12 to 21)
	18:00 – 19:00	Dinner
	19:00 – 22:00	Poster Session II (Posters 12 to 21)

Thursday, 17.09.2026		
	08:00 – 09:00	Breakfast
Session 14 Chair: Martina Havenith	09:00 – 10:00	Marialore Sulpizi <i>Machine Learning in Nanoconfinement: Pushing the Limits of Time</i>
	10:00 – 11:00	Arne Lützen <i>Chemistry of and in Metallosupramolecular Cages</i>
	11:00 – 11:30	Coffee Break
Session 15 Chair: Lars Schäfer	11:30 – 12:30	Roland Netz <i>Friction and transport in nanoconfined water and electrolytes</i>
	12:30 – 13:00	Closing Remarks - Karina Morgenstern
	13:00 – 14:30	Lunch
	14:30	Departure

Summarized agenda. Invited talks in yellow, contributed talks in blue, flash talks and poster sessions in green.

	Sun, 13.09.2026	Mon, 14.09.2026	Tue, 15.09.2026	Wed, 16.09.2026	Thu, 17.09.2026
08:00	Arrival	Breakfast	Breakfast	Breakfast	Breakfast
09:00		Paul Lusby	Marie-Pierre Gageot	Cheng-Yong Su	Marialore Sulpizi
10:00		Gregori Ujaque	Shadi Fatayer	Venkat Kapil	Arne Lützen
11:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:30		Joost Reek	Katrin Domke	Ebba Matic	Roland Netz
12:30		Irina Cuesta Lucas Araujo	Bashar Moussa WE-Heraeus F.	Luca M. Sicking Mandy Hoffmann	Closing Remarks
13:00		Lunch	Lunch	Photo + Lunch	Lunch
14:30		Hannah Kurz	Antonio M.-Martínez Aleksandr Mikherdov	Sofia Kolin	Departure
15:00		Kai Zhang Maya Heine	Excursion	Qixuan Li Johannes Fiedler	
15:30				Coffee Break	
16:00	Check-in	Coffee Break		Malte Feßner Mingkai Zhao	
16:30	Opening Remarks	Laurie Stevens Russell Kajouri		Flash Talks II	
17:00	Jennifer MacLeod	Flash Talks I		Dinner	
18:00	Buffet Supper	Dinner		Poster Session II	
19:00	Niels Hansen	Poster Session I	Heraeus Dinner		
20:00					
21:00					

Poster number	Presenter
01	Mercè Alemany Chavarria <i>Computational study of guest behaviour inside a metallobox</i>
02	Malte Feßner <i>Site-effects in matrix isolation investigated with multidimensional IR spectroscopy</i>
03	Laura Schneider <i>Donor-Acceptor Self-Assembled Co(III) Supramolecular Bowls for Photoinduced Charge Separation</i>
04	Yifan Li <i>Huisgen Cycloaddition Reactions in Poly-imine Bis-calix[4]pyrrole Cages: Balancing Acceleration, Regioselectivity, and Turnover</i>
05	Luciana Herbeck <i>How external stimuli trigger the release of the secondary messenger NO from confined matrixes</i>
06	Matthias-Julian Justen <i>Encapsulation of C2-symmetric guests in metallosupramolecular aggregates for enantioselective catalysis</i>
07	Simon Knüver <i>Dissecting the Driving Forces Behind Heteroleptic Coordination Cages Formation</i>
08	Abhinu Menoth Sasisharan <i>Stimuli-responsive reversible guest exchange cycles in a charge-neutral metal helicate</i>
09	Andriana Loukovitou <i>Confinement-controlled ultrafast fs laser induced synthesis of bi- and multimetallic nanoparticles</i>
10	Xiaochen Yang <i>Effects of Pd-Capping Ligands on Dynamic Behaviors within Pd₆L₄¹²⁺ Metal–Organic Cages</i>
11	Anne Müller-Feyen <i>Light-fuelled metal-organic cages from bistable to transient states</i>
12	Ashley Stingel <i>Tracking Photoinduced Proton Transfer Inside Reverse Micelles</i>
13	Yannick Weidemann <i>Covalent Organic Framework Induced Confinement of Hydrogen-Bonded Water</i>
14	Hannah Wessely <i>Energy Transfer Between BODIPY-Derivatives in Pd₂L₄ Cages</i>
15	Björn Schmidt <i>Confining Molecular Motor in Palladium-based Self-assemblies</i>
16	Veronika Stoianova <i>Azobenzene photo-switching investigation under confined conditions using chiroptical spectroscopy tools</i>
17	Aiswarya Roby <i>Metallo-Salen-based Self-Assembled Rings</i>
18	Cagri Turan <i>Exploring supramolecular rings by scanning tunneling microscopy</i>
19	Lars Hebenbrock <i>Coordination Cages based on Photoredox Catalysts</i>
20	Iqra Yousaf <i>Isotopic Fingerprints of Excess Proton Transfer Dynamics in Aqueous Solution by THz/IR Spectroscopy</i>
21	Min Zou <i>Computational Investigation of Electric Field Effects in Metallocages</i>