

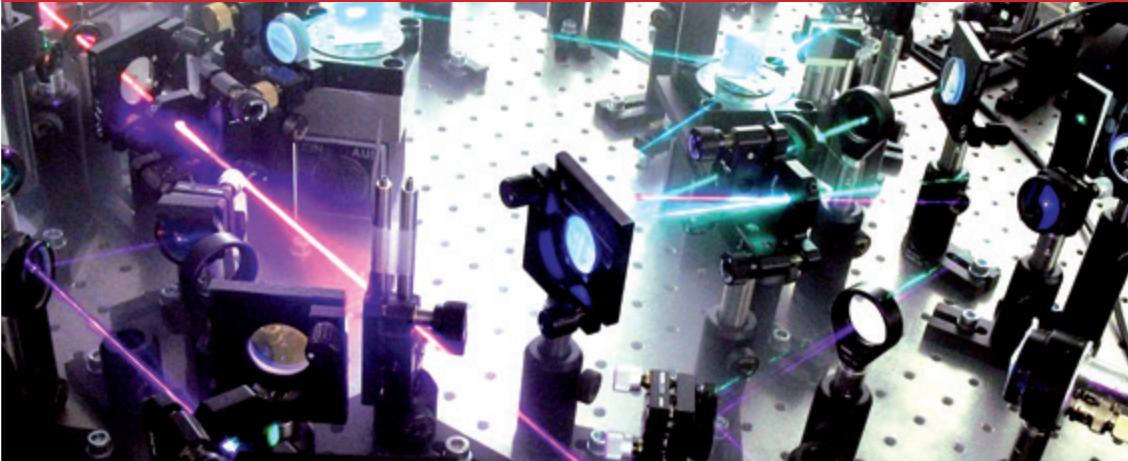
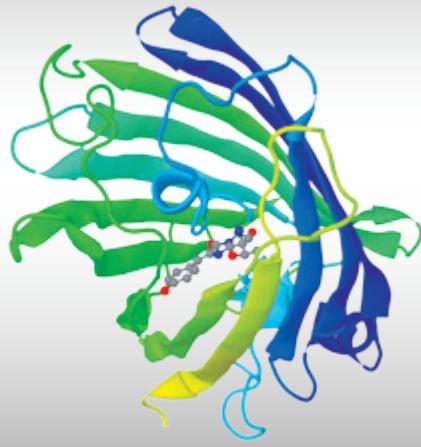


# BUNSENTAGUNG 2017

## 116<sup>th</sup> General Assembly of the German Bunsen Society for Physical Chemistry

Featuring an industrial symposium with accompanying exhibition  
and Karriereforum

25 – 27 May 2017 · Kaiserslautern · Germany



## PROGRAMME

## Physical Chemistry for Life Sciences

[www.bunsentagung.de](http://www.bunsentagung.de)



 TECHNISCHE UNIVERSITÄT  
KAISERSLAUTERN



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The picture on the lower half of the cover illustrates a fluorescence microscopy image of Purkinje cells (green) including counterstaining (Hoechst, blue) in the mouse cerebellum. The organisers sincerely thank Prof. Dr. Kins and his working group (TU Kaiserslautern, Department of Biology) who made this image available.

**MAIN TOPIC:**

## “Physical Chemistry for Life Sciences”

The tremendous progress in Life Sciences that brought this discipline into the public spotlight in the last decades has been spurred by the development and refinement of methods from both experimental and theoretical physical chemistry. The contribution of physical chemistry to Life Sciences as a key technology of the 21<sup>st</sup> century must not be underestimated and strongly enabled the analysis of biologically relevant processes on a molecular level. This is e.g. a precondition for medical science to design drugs and therapeutic approaches.

Some methodological developments like matrix-assisted laser desorption/ionization (MALDI) and electrospray ionization (ESI) paved the way for mass spectrometry to become a standard analytical technique in proteomics. Furthermore spectroscopy and microscopy yield information on structure, functionality and whole biological processes in the disciplines of Life Sciences. Manifold spectroscopic techniques exist which are able to cover different sizes of molecular systems in gas and condensed phase and with respect to different time resolutions. Due to the complexity of biological systems e.g. a bottom-up approach can start with the investigation of single molecular components. In this context different (laser) spectroscopic techniques for example analyze isolated species in molecular beams or ion traps yielding intrinsic structural properties with regard to fundamental interactions like hydrogen bonds, dispersion or electrostatic stabilization. Those kinds of interactions also govern intermediate structures in protein folding pathways or are important in rational drug design for specific biomolecular targets. In addition time resolved spectroscopy reaching from millisecond to femtosecond resolution allows to activate, probe and analyze energy levels and thereby to follow dynamics of biologically relevant systems of different sizes. The structure elucidation of macromolecules like proteins, lipids, DNA or RNA as well as macromolecular complexes is also a domain of EPR and NMR spectroscopy. Further increasing in size the visualization of cellular structures or whole cells is the domain of microscopy though (especially with regard to fluorescence) the junction to spectroscopy is fluent.

Despite this enormous pool of techniques – only a few were addressed here – theoretical studies are necessary to gain insight into processes of biological systems on a molecular level and by this to interpret and support experimental findings. Depending on the size of the system advanced *ab initio* and DFT-based chemical methods or molecular dynamics simulations are applied with the latter even allowing the analysis of large biological entities (e.g. proteins, ion channels, membranes).

As briefly illustrated above the application of physical chemistry concepts and methods branches out in fields of biochemistry, molecular biology, molecular medicine and should in this meeting bring together outstanding scientists to discuss leading-edge results and push the frontiers of these fields further. The strong interdisciplinary aspect of the main topic of the Bunsentagung 2017 should foster discussions and spawn new collaborations across the boundaries of scientific disciplines.

**COMMITTEE / ORGANISATION****PROGRAMME COMMITTEE**

<b>Nadja Carola Bigall</b>	Universität Hannover/D	<b>Christoph Riehn</b>	TU Kaiserslautern/D
<b>Bernhard Dick</b>	Universität Regensburg /D	<b>Joachim Sauer</b>	Humboldt-Universität zu Berlin/D
<b>Rolf Diller</b>	TU Kaiserslautern/D	<b>Rolf Schäfer</b>	TU Darmstadt/D
<b>Markus Gerhards</b>	TU Kaiserslautern/D	<b>Claus A.M. Seidel</b>	Heinrich-Heine-Universität Düsseldorf/D
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<b>Gereon Niedner-Schatteburg</b>	TU Kaiserslautern/D	<b>Christoph van Wüllen</b>	TU Kaiserslautern/D
<b>Christian Ochsenfeld</b>	LMU München/D		

**LOCAL AND SCIENTIFIC ORGANISERS**

<b>Markus Gerhards</b>	TU Kaiserslautern/D	<b>Christoph Riehn</b>	TU Kaiserslautern/D
<b>Gereon Niedner-Schatteburg</b>	TU Kaiserslautern/D	<b>Marc Prosenc</b>	TU Kaiserslautern/D
<b>Christoph van Wüllen</b>	TU Kaiserslautern/D	<b>Kirsten Schwing</b>	TU Kaiserslautern/D
<b>Rolf Diller</b>	TU Kaiserslautern/D		

**HOST**

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## EXHIBITION & SPONSORING

Companies are invited to participate in the accompanying exhibition. The exhibition presents a perfect opportunity to inform participants about your products and services as well as for networking. There are also various sponsoring opportunities available.

If you are interested in either exhibiting or sponsoring, please contact the the Bunsen Society (geschaeftsstelle@bunsen.de).

### LIST OF EXHIBITORS

(as of 10 February 2017)

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(as of 10 February 2017)

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### FURTHER FINANCIAL SUPPORT

(as of 10 February 2017)

- **State Research Center OPTIMAS**, Kaiserslautern/D
- **SFB - 3MET**, Kaiserslautern/D
- **Evonik Industries AG**, Essen/D
- **Technische Universität Kaiserslautern**, Kaiserslautern/D

## PROGRAMME AT A GLANCE

## Thursday, 25 May 2017

11:30-14:30	<b>Karriereforum</b> (in German only)	
15:00	<b>Ordentliche Mitgliederversammlung</b> (nur für Mitglieder der DBG, in German only)	
16:30-18:15	Audimax	<b>OPENING CEREMONY</b>
18:15-19:00		<b>OPENING LECTURE:</b> Mann
19:15-22:30	Mensa	<b>Welcome Reception</b>

## Friday, 26 May 2017

Chair	van Wüllen							
08:30-09:10	<b>Audimax</b>	<b>PLENARY LECTURE:</b> Prisner						
	<b>Audimax 42-115</b>	<b>HS 42-110</b>		<b>HS 46 - 220</b>	<b>HS 46 - 215</b>	<b>HS 46 - 210</b>		
	<b>Main Topic</b>	<b>Main Topic</b>		<b>Surfaces and Interfaces</b>	<b>Solids and Nano-sized Matter</b>	<b>Industrial Applications</b>		
Chair	Meister	von Helden		Kartouzian	Dorfs	Rieger		
09:25-09:45	Frosch	Mons		Paier	Heinke	Votsmeier		
09:45-10:05	Thallmair	Pagel		Thissen	Weippert	Künkel		
10:05-10:25	Menges	Na		Zurhelle	Genreith-Schriever	Franke		
10:25-10:45	Mutas	Villatoro		Park	Scheele	Kortz		
10:45-11:05	COFFEE BREAK							
	<b>Main Topic</b>	<b>Main Topic</b>		<b>Surfaces and Interfaces</b>	<b>Solids and Nano-sized Matter</b>	<b>Industrial Applications</b>		
Chair	Kottke	Kruss		R. Schäfer	Chanaewa	Thaler		
11:05-11:25	Peulen	Horke		Sanchez	Bigall	Wünsche		
11:25-11:45	Tripathi	Boyarkine		Ruiz-Barragan	Boldt	Kessler		
11:45-12:05	Blank	Gutmann		Hein	Hofmann	Plass		
12:05-13:05	LUNCH BREAK							
Chair:	Seidel							
13:05-13:45	<b>Audimax</b>	<b>PLENARY LECTURE:</b> Schwille						
13:45-14:25	<b>Audimax</b>	<b>PLENARY LECTURE:</b> Motzkus						
	<b>Audimax 42-115</b>	<b>HS 42-110</b>		<b>HS 46 - 220</b>	<b>HS 46 - 215</b>	<b>HS 46 - 210</b>		
	<b>Main Topic</b>	<b>Award Session/ Funding Symposium</b>		<b>Surfaces and Interfaces</b>	<b>Solids and Nano-sized Matter</b>	<b>Molecular Structure</b>		
Chair	Winter	Nickel		Park	Bigall	Schooss		
14:40-15:00	Garidel	Ewald-Wicke		Kelly	Lauth	Fatima		
15:00-15:20	Müh	Nernst-Haber-Bodenstein		Stöckl	Stroyuk	Bernhard		
15:20-15:40	Niether	Wachter (DFG)		Lach	Guhrenz	Pérez de Tudela		
15:40-16:00	Huber			Prosenc	Niedermaier	Strelnikov		
16:00-16:20	COFFEE BREAK							
	<b>Main Topic</b>	<b>Main Topic</b>		<b>Theoretical Techniques</b>	<b>Experimental Techniques</b>	<b>Molecular Structure</b>		
Chair	Blank	Bald		Paier	Merk	Suhm		
16:20-16:40	Eberl	Dietzek		Burow	Endres	Schooss		
16:40-17:00	Pierik	Calandrini		Jagau	Dopfer	Krüger		
17:00-17:20	Wiegand	von Helden		Springborg	Obenchain	Debnath		
17:20-17:40	Chowdhury	Forsting		Kühne	Patra	Niemann		
17:40-18:00	Müller-Werkmeister	Meister		Kats	Dörr	Gradzielski		
	Mensa							
18:15-19:45	<b>POSTER SESSION:</b> (even numbers)							
19:45-21:15	<b>POSTER SESSION:</b> (odd numbers)							

## Saturday, 27 May 2017

		Gerhards					
08:30-09:10		Audimax	PLENARY LECTURE: Rizzo				
		Audimax 42-115	HS 42-110	HS 46 - 220	HS 46 - 215	HS 46 - 210	HS 46 - 110
		Main Topic	Main Topic	Liquids and Solvation	Solids and Nano-sized Matter	Chemical Dynamics and Kinetics	Electrochemistry and Energy
Chair	Heberle	Niedner-Schatteburg	Ludwig	Lauth	Riehn	Marschall	
09:25-09:45	Möller	Fuji	Vondracek	Klinke	Straub	Lenzer	
09:45-10:05	Gao	Nieto	Vila Verde	Dorfs	Reiffers	Kim	
10:05-10:25	van Wilderen	Müller	Muñoz-Santiburcio	Mohrhusen	Nuernberger	Brummel	
10:25-10:45	Ebbinghaus	Heid	Sebastiani	Wuttke	Vöhringer	Cai	
10:45-11:05	COFFEE BREAK						
		Main Topic	Main Topic	Liquids and Solvation	Catalysis	Chemical Dynamics and Kinetics	Surfaces and Interfaces
Chair	Diller	Keller	Sebastiani	Hofmann	Landgraf	Boldt	
11:05-11:25	Full Lecture	König	Strate	Winterlin	Höveler	Klein	
11:25-11:45	Heberle	Klossek	Kerlé	Klyushin	Meyer	Buller	
11:45-12:05	Grethen	Bald	Rathke	Yu	Winghart	Schmid	
12:05-12:25	Drücker	Khadem	Golub	Moskaleva	Ončák	Antonsson	
12:25-13:30	LUNCH BREAK						
Chair	Küpper						
13:30-14:10		Audimax	PLENARY LECTURE: Grubmüller				
		Audimax 42-115	HS 42-110	HS 46 - 220	HS 46 - 215	HS 46 - 210	HS 46 - 110
		Main Topic	Main Topic	Liquids and Solvation	Catalysis	Chemical Dynamics and Kinetics	Hot Topic
Chair	Gutmann	Ebbinghaus	Vila Verde	Winterlin	Nürnberg	Horke	
14:25-14:45	Engelke	Kutta	Vogler	Lang	Tschierlei	Greisch	
14:45-15:05	Brand	Meister	Fischer	Kunz	Oum	Weitzel	
15:05-15:25	Schulze	Kottke	Huggins	Ristig	Landgraf	Kramer	
15:25-15:45	Keller	Berger	Gleim	Hemberger	Megow	Niefind	
16:00-16:30	Poster Awards and Closing Session						

OPENING LECTURE / PLENARY LECTURES**OPENING LECTURE****Thursday, 25 May 2017**

- 18:15 – 19:00 **Development of Proteomics Technologies and their Application to Life Sciences**  
Matthias Mann, Max-Planck-Institute of Biochemistry, Martinsried/D

**PLENARY LECTURES****Friday, 26 May 2017**

- 8:30 – 9:10 **Structure and Conformational Dynamics of Biomolecules Investigated by Pulsed EPR**  
Thomas Prisner, Goethe University Frankfurt/D
- 13:05 – 13:45 **Towards a Smallest Unit of Life**  
Petra Schwille, Max-Planck-Institute of Biochemistry, Martinsried/D
- 13:45 – 14:25 **Quantum Control (micro-) Spectroscopy: Studying Biomolecules with Complex Laser Pulses**  
Marcus Motzkus, Heidelberg University/D

**Saturday, 27 May 2017**

- 8:30 – 9:10 **New Dimensions in Biomolecular Mass Spectrometry and Ion Spectroscopy**  
Thomas Rizzo, Ecole Polytechnique Fédérale de Lausanne/CH
- 13:30 – 14:10 **Forces and Conformational Dynamics in Biomolecular Nanomachines**  
Helmut Grubmüller, Max-Planck-Institute of Biophysical Chemistry, Göttingen/D

## MEETINGS OF THE GERMAN BUNSEN SOCIETY

## Thursday, 25 May 2017

09:00 – 11:00	<b>Vorstandssitzung*</b> (only invitational)	Room 44-482
09:00 – 11:00	<b>Sitzung der Themenkommission*</b>	Room 44-465
11:00 – 13:30	<b>Sitzung des Ständigen Ausschusses*</b> (only invitational)	Room 44-380
11:30 – 14:30	<b>Karriereforum* „Forschung nach der Promotion“</b>	Room 42-110
13:30 – 15:00	<b>Sitzung der Studienkommission*</b>	Room 42-105
15:00 – 16:00	<b>Ordentliche Mitgliederversammlung*</b> (only for DBG members)	Room 42-110

## Friday, 26 May 2017

12:05 – 13:05	<b>Women's Networking Lunch</b>	Room 46-267
<b>Saturday, 27 May 2017</b>		
12:30 – 13:30	<b>Mitgliederversammlung AG Bunsen-Karriereforum*</b>	Room 46-267

\* in German only

## LECTURE PROGRAMME

## Thursday, 25 May 2017

	HS 42-110
11:30-14:30	Karriereforum (in German only)
15:00	Ordentliche Mitgliederversammlung (nur für Mitglieder der DBG, in German only)
	Audimax HS 42-115
16:30-18:15	OPENING CEREMONY
18:15-19:00	<b>OPENING LECTURE</b> Development of Proteomics Technologies and their Application to Life Sciences Matthias Mann, Max-Planck-Institute of Biochemistry, Martinsried/D
	Mensa (Gebäude 30)
19:15-22:30	Welcome Reception

## LECTURE PROGRAMME

Friday, 26 May 2017

Morning

	Room: Audimax: 42-115	
Chair	<i>C. van Wüllen, TU Kaiserslautern</i>	Chair
08:30	<b>PLENARY LECTURE</b> <b>Structure and Conformational Dynamics of Biomolecules Investigated by Pulsed EPR</b> <u>T. Prisner</u> <sup>1</sup> ; <sup>1</sup> Universität Frankfurt am Main/D	08:30
	Room: Audimax: 42-115	Room: HS 42-110
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Main Topic - Physical Chemistry for Life Sciences</b>
Chair	<i>A. Meister, Universität Halle-Wittenberg/D</i>	<i>G. von Helden, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D</i>
09:25	<b>Monitoring life science processes by Raman gas spectroscopy</b> <u>T. Frosch</u> <sup>1</sup> ; <sup>1</sup> T. Jochum <sup>1</sup> ; <sup>1</sup> J. Popp <sup>1</sup> ; <sup>1</sup> Leibniz-Institut für Photonische Technologien, Jena/D	Local anchoring of asparagine side chains to the protein backbone: gas phase laser spectroscopy as a benchmark for understanding the turn promoting behavior of Asn <u>S. Habka</u> <sup>1</sup> ; <sup>1</sup> Y. Sohn <sup>1</sup> ; <sup>1</sup> V. Vaquero-Vara <sup>1</sup> ; <sup>1</sup> M. Géleoc <sup>1</sup> ; <sup>1</sup> B. Tardivel <sup>1</sup> ; <sup>1</sup> V. Brenner <sup>1</sup> ; <sup>1</sup> E. Gloaguen <sup>1</sup> ; <sup>1</sup> M. Mons <sup>2</sup> ; <sup>1</sup> CEA CNRS Université Paris Saclay, Gif-sur-Yvette/F; <sup>2</sup> CEA Commissariat à l'Energie Atomique, Gif-sur-Yvette/F
09:45	<b>The impact of cholesterol flip-flop on the plasma membrane – insights from simulations</b> <u>S. Thallmair</u> <sup>1</sup> ; <sup>1</sup> H. Ingólfsson <sup>2</sup> ; <sup>1</sup> S. Marrink <sup>1</sup> ; <sup>1</sup> University of Groningen/ NL; <sup>2</sup> Lawrence Livermore National Laboratory/USA	<b>An Infrared Spectroscopy Approach to Follow β-Sheet Formation in Peptide Amyloid Assemblies</b> <u>J. Seo</u> <sup>1</sup> ; <sup>1</sup> W. Hoffmann <sup>2</sup> ; <sup>1</sup> S. Warnke <sup>1</sup> ; <sup>1</sup> X. Huang <sup>1</sup> ; <sup>1</sup> S. Gewinner <sup>1</sup> ; <sup>1</sup> W. Schöllkopf <sup>1</sup> ; <sup>1</sup> M. Bowers <sup>3</sup> ; <sup>1</sup> G. von Helden <sup>1</sup> ; <sup>1</sup> K. Pagel <sup>2</sup> ; <sup>1</sup> Fritz Haber Institute of the Max Planck Society, Berlin/D; <sup>2</sup> Freie Universität Berlin, Institut für Chemie und Biochemie, Organische Chemie, Berlin/D; <sup>3</sup> University of California, Santa Barbara/USA
10:05	<b>Multi-emissive Molecular Probes in Medical Diagnosis</b> <u>J. Menges</u> <sup>1</sup> ; <sup>1</sup> B. Finkler <sup>1</sup> ; <sup>1</sup> G. Jung <sup>1</sup> ; <sup>1</sup> Saarland University, Saarbrücken/D	<b>Molecular dynamics simulation of electron transfer reactions: from single proteins to protein aggregates</b> <u>S. Na</u> <sup>1</sup> ; <sup>1</sup> A. Bauß <sup>1</sup> ; <sup>1</sup> T. Koslowski <sup>1</sup> ; <sup>1</sup> University of Freiburg/D
10:25	<b>Fluorescent Gold Nanoparticles on/in Cells Visualized by Fluorescence-Lifetime Imaging Microscopy</b> <u>M. Mutas</u> <sup>1</sup> ; <sup>1</sup> Universität Hamburg/D	<b>Low and High Field Mobilities determined by IR-MALDI Ion Mobility Spectrometry at Intermediate Pressure</b> <u>J. Villatoro</u> <sup>1</sup> ; <sup>1</sup> Universität Potsdam/Physikalische Chemie/D
10:45	COFFEE BREAK	
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Main Topic - Physical Chemistry for Life Sciences</b>
Chair	<i>T. Kottke, Universität Bielefeld/D</i>	<i>S. Kruss, Universität Göttingen/D</i>
11:05	<b>Simulating fluorescence from picosecond to milliseconds to map dynamics and macromolecular structure in solution</b> <u>T. Peulen</u> <sup>1</sup> ; <sup>1</sup> C. Hengstenberg <sup>2</sup> ; <sup>1</sup> M. Dimura <sup>1</sup> ; <sup>1</sup> A. Valeri <sup>1</sup> ; <sup>1</sup> H. Gohlke <sup>1</sup> ; <sup>1</sup> C. Herrmann <sup>2</sup> ; <sup>1</sup> C. Seidel <sup>1</sup> ; <sup>1</sup> Heinrich-Heine-Universität, Düsseldorf/D; <sup>2</sup> Ruhr-Universität, Bochum/D	<b>Controlling the motion of very large molecules and particles</b> <u>D. Horke</u> <sup>1</sup> ; <sup>1</sup> S. Awel <sup>1</sup> ; <sup>1</sup> D. Gusa <sup>2</sup> ; <sup>1</sup> Z. Huang <sup>1</sup> ; <sup>1</sup> T. Ossenbrüggen <sup>2</sup> ; <sup>1</sup> N. Roth <sup>2</sup> ; <sup>1</sup> I. Rubinsky <sup>2</sup> ; <sup>1</sup> A. Samantha <sup>2</sup> ; <sup>1</sup> V. Singh <sup>2</sup> ; <sup>1</sup> X. Sun <sup>2</sup> ; <sup>1</sup> N. Teschmit <sup>1</sup> ; <sup>1</sup> L. Worbs <sup>2</sup> ; <sup>1</sup> J. Küpper <sup>3</sup> ; <sup>1</sup> Center for Free-Electron Laser Science, DESY, Hamburg/D; <sup>2</sup> Center for Free-Electron Laser Science, DESY, Hamburg/D; <sup>3</sup> Center for Free-Electron Laser Science, DESY, The Hamburg Centre for Ultrafast Imaging, Hamburg/D
11:25	<b>Molecular-Level Insights into the Catalytic Mechanism of Human Guanylate-Binding Protein 1 (hGBP1) from Accelerated QM/MM Simulations</b> <u>R. Tripathi</u> <sup>1</sup> ; <sup>1</sup> R. Glaves <sup>1</sup> ; <sup>1</sup> D. Marx <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	<b>Critical assessment and new developments for Cold Ion Spectroscopy of biomolecules</b> <u>V. Kopysov</u> <sup>1</sup> ; <sup>1</sup> <u>O. Boyarkine</u> <sup>1</sup> ; <sup>1</sup> EPFL, Lausanne/CH
11:45	<b>Molecular Mechanics of Coiled Coil Crosslinked Hydrogels</b> <u>A. Sanz de León</u> <sup>1</sup> ; <sup>1</sup> M. Goktas <sup>1</sup> ; <sup>1</sup> P. López García <sup>1</sup> ; <sup>1</sup> K. Blank <sup>1</sup> ; <sup>1</sup> Max Planck Institute of Colloids and Interfaces, Potsdam/D	<b>Functional Materials for Life Science Applications – Spins as Spies for Characterization of Local Structures</b> <u>T. Gutmann</u> <sup>1</sup> ; <sup>1</sup> Technische Universität Darmstadt/D
12:05	LUNCH BREAK	
	12:05	

Friday, 26 May 2017

Morning

	Room: Audimax: 42-115	
Chair	C. van Wüllen, TU Kaiserslautern	Chair
08:30	<b>PLENARY LECTURE</b> <b>Structure and Conformational Dynamics of Biomolecules Investigated by Pulsed EPR</b> <u>T. Prisner</u> <sup>1</sup> ; <sup>1</sup> Universität Frankfurt am Main/D	08:30
	Room: HS 46-220	Room: HS 46-215
	<b>Surfaces and Interfaces</b>	<b>Solids and Nano-sized Matter</b>
Chair	A. Kartouzian, TU München/D	D. Dorfs, Universität Hannover/D
09:25	<b>A DFT snapshot on the dynamic iron oxide exposed to water: What we can learn from model studies</b> J. Paier <sup>1</sup> ; X. Li <sup>1</sup> ; <sup>1</sup> Humboldt-Universität zu Berlin/D	<b>Thin Films of Photoswitchable Metal-Organic Frameworks</b> <u>L. Heinke</u> <sup>1</sup> ; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
09:45	<b>Mechanism of Phosphorus Transport through Silicon Oxide</b> R. Longo <sup>1</sup> ; E. Mattson <sup>2</sup> ; N. Giraudo <sup>3</sup> ; S. Rupich <sup>1</sup> ; K. Cho <sup>1</sup> ; Y. Chabal <sup>1</sup> ; P. Thissen <sup>3</sup> ; <sup>1</sup> University of Texas at Dallas, Richardson/USA; <sup>2</sup> University of Texas at Dallas, Richardson/USA; <sup>3</sup> Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Eggenstein-Leopoldshafen/D	<b>Dimerization process in Coronene films</b> <u>J. Weippert</u> <sup>1</sup> ; J. Bachmann <sup>1</sup> ; J. Greisch <sup>1</sup> ; A. Böttcher <sup>1</sup> ; M. Kappes <sup>1</sup> ; <sup>1</sup> KIT Karlsruhe/D
10:05	<b>Surface defect chemistry of Ceria: A Poisson–Cahn Treatment</b> A. Zurbelle <sup>1</sup> ; X. Tong <sup>2</sup> ; R. De Souza <sup>1</sup> ; D. Mebane <sup>3</sup> ; <sup>1</sup> Institute of Physical Chemistry, RWTH Aachen University/D; <sup>2</sup> West Virginia University, Morgantown/USA; <sup>3</sup> West Virginia University, Morgantown/D	<b>Field-enhanced Ion Transport Revisited</b> <u>A. Genreith-Schriever</u> <sup>1</sup> ; R. De Souza <sup>1</sup> ; <sup>1</sup> RWTH Aachen University/D
10:25	<b>Scattering Formaldehyde from the Au(111) Surface</b> B. Park <sup>1</sup> ; B. Krüger <sup>2</sup> ; S. Meyer <sup>2</sup> ; A. Wodtke <sup>2</sup> ; T. Schäfer <sup>2</sup> ; <sup>1</sup> Georg-August-Universität Göttingen/D; <sup>2</sup> Georg-August-Universität Göttingen, Institute of Physical Chemistry/D	<b>Monitoring the Formation of Conductive PbS Nanocrystal Superlattices at the Liquid/Air Interface in Real Time by X-ray Scattering</b> A. André <sup>1</sup> ; S. Maiti <sup>1</sup> ; J. Hagenlocher <sup>1</sup> ; F. Schreiber <sup>1</sup> ; R. Banerjee <sup>1</sup> ; M. Scheele <sup>1</sup> ; <sup>1</sup> Eberhard Karls Universität Tübingen/D
10:45	COFFEE BREAK	
	<b>Surfaces and Interfaces</b>	<b>Solids and Nano-sized Matter</b>
Chair	R. Schäfer, TU Darmstadt/D	A. Chanaewa, Universität Freiburg/D
11:05	<b>Surface melting of ice</b> M. Sánchez <sup>1</sup> ; M. van Zadel <sup>1</sup> ; J. Cyran <sup>1</sup> ; P. Sudera <sup>1</sup> ; Y. Nagata <sup>1</sup> ; M. Bonn <sup>1</sup> ; E. Backus <sup>1</sup> ; <sup>1</sup> Max Planck Institute for Polymer Research, Mainz/D	<b>Functional 3D Assemblies of Nanoparticles</b> <u>A. Freytag</u> <sup>1</sup> ; S. Naskar <sup>1</sup> ; F. Lübemann <sup>1</sup> ; J. Miethe <sup>1</sup> ; <u>N. Bigall</u> <sup>1</sup> ; <sup>1</sup> Leibniz Universität Hannover/D
11:25	<b>Graphene-water interactions: A new electronic-structure-based force field</b> S. Ruiz-Barragan <sup>1</sup> ; D. Muñoz-Santibucio <sup>1</sup> ; D. Marx <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	<b>Effects of Grading in Core/Shell/Shell Quantum Dots</b> P. Zeng <sup>1</sup> ; F. Enders <sup>2</sup> ; T. Smith <sup>1</sup> ; <u>K. Boldt</u> <sup>2</sup> ; <sup>1</sup> University of Melbourne/AUS; <sup>2</sup> Universität Konstanz/D
11:45	<b>Electro-diffusion versus chemical diffusion in alkali calcium phosphate glasses – implication of structural changes</b> <u>A. Hein</u> <sup>1</sup> ; J. Martin <sup>1</sup> ; M. Schäfer <sup>1</sup> ; K. Weitzel <sup>1</sup> ; <sup>1</sup> Philipps-Universität Marburg/D	<b>Sub-second charge carrier dynamics in TiO<sub>2</sub> photocatalysts studied by time-resolved FTIR: influence of surface hydration</b> A. Litke <sup>1</sup> ; T. Weber <sup>1</sup> ; E. Hensen <sup>1</sup> ; <u>J. Hofmann</u> <sup>1</sup> ; <sup>1</sup> TU Eindhoven/NL
12:05	LUNCH BREAK	

## LECTURE PROGRAMME

Friday, 26 May 2017

Morning

	Room: Audimax: 42-115	
Chair	C. van Wüllen, TU Kaiserslautern	Chair
08:30	<b>PLENARY LECTURE</b> <b>Structure and Conformational Dynamics of Biomolecules Investigated by Pulsed EPR</b> <u>T. Prisner</u> <sup>1</sup> ; <sup>1</sup> Universität Frankfurt am Main/D	08:30
	Room: HS 46-210	Room: HS 46-110
	<b>Industrial Applications</b>	<b>Chemical Dynamics and Kinetics</b>
Chair	J. Rieger, BASF SE, Ludwigshafen/D	J. Meyer, Universität Innsbruck/A
09:25	Low temperature exhaust catalysis: Short pulse reductive activation of Pt/CeO <sub>2</sub> B. Betz <sup>1</sup> ; M. Votsmeier <sup>2</sup> ; R. Hoyer <sup>2</sup> ; A. Wörz <sup>2</sup> ; <sup>1</sup> TU Darmstadt/D; <sup>2</sup> Umicore AG & Co. KG, Hanau-Wolfgang/D	Effect of the carbonyl group in the oxidation of small methyl ketones C. Hemken <sup>1</sup> ; U. Burke <sup>2</sup> ; J. Pieper <sup>1</sup> ; R. Büttgen <sup>2</sup> ; K. Heufer <sup>2</sup> ; K. Kohse-Höinghaus <sup>1</sup> ; <sup>1</sup> Bielefeld University/D; <sup>2</sup> RWTH Aachen University/D
09:45	Certified biodegradable mulch film – Ecological benefits and environmental fate A. Künkel <sup>1</sup> ; <sup>1</sup> BASF SE, Ludwigshafen/D	Auto-ignition of Diethyl Ether: Development of a Mechanism and Kinetic Modeling J. Eble <sup>1</sup> ; J. Kiecherer <sup>1</sup> ; C. Bänsch <sup>1</sup> ; M. Olzmann <sup>1</sup> ; <sup>1</sup> Karlsruher Institut für Technologie (KIT), Institut für Physikalische Chemie/D
10:05	Investigations into kinetic and mechanistic aspects of hydroformylation R. Franke <sup>1</sup> ; <sup>1</sup> Evonik Performance Materials GmbH, Marl/D	Systematische Untersuchung von H-Abstraktionsreaktionen in laminaren Niederdruckflammen mittels Photoelektronen-Photoionen-Koinzidenz-Spektroskopie (PEPICO). D. Krüger <sup>1</sup> ; M. Köhler <sup>1</sup> ; P. Oßwald <sup>1</sup> ; T. Bierkandt <sup>2</sup> ; Y. Karakaya <sup>2</sup> ; P. Hemberger <sup>3</sup> ; T. Kasper <sup>2</sup> ; <sup>1</sup> German Aerospace Center (DLR), Stuttgart/D; <sup>2</sup> Universität Duisburg-Essen/D; <sup>3</sup> Paul Scherrer Institut (PSI), Villigen/CH
10:25	Electrochromic Iris for Low-space and Low-power Optical Applications C. Kortz <sup>1</sup> ; E. Oesterschulze <sup>1</sup> ; <sup>1</sup> TU Kaiserslautern/D	Femtosecond dynamics of the 2-methylallyl radical in the gas phase A. Röder <sup>1</sup> ; I. Fischer <sup>1</sup> ; R. Mitric <sup>1</sup> ; L. Poisson <sup>2</sup> ; J. Petersen <sup>1</sup> ; K. Issler <sup>1</sup> ; M. Wohlgemuth <sup>1</sup> ; <sup>1</sup> Julius Maximilians University of Würzburg/D; <sup>2</sup> CEA Saclay, Gif-sur-Yvette/F
10:45	COFFEE BREAK	10:45
	<b>Industrial Applications</b>	<b>Hot Topic</b>
Chair	A. Thaler, 3M/Dyneon GmbH, Burgkirchen/D	J.-U. Grabow, Universität Hannover/D
11:05	Laser systems for resonance ionization sources for isotope separator facilities P. Jauernik <sup>1</sup> ; A. Wloka <sup>1</sup> ; C. Wünsche <sup>1</sup> ; <sup>1</sup> Sirah Lasertechnik GmbH, Grevenbroich/D	Photoacoustic measurements of photokinetics in single optically trapped aerosol droplets J. Cremer <sup>1</sup> ; P. Covert <sup>1</sup> ; R. Signorelli <sup>1</sup> ; K. Thaler <sup>2</sup> ; C. Haisch <sup>2</sup> ; <sup>1</sup> ETH Zürich/CH; <sup>2</sup> Technische Universität München, D
11:25	Time resolved FTIR spectroscopic techniques – Insights into reactions and kinetics M. Kessler <sup>1</sup> ; D. Czurlok <sup>1</sup> ; M. Jörger <sup>1</sup> ; <sup>1</sup> Bruker Optik GmbH, Ettlingen/D	The dynamics of active metal catalysts revealed by <i>in situ</i> electron microscopy M. Willinger <sup>1</sup> ; J. Cao <sup>1</sup> ; A. Rinaldi <sup>1</sup> ; Z. Wang <sup>1</sup> ; M. Greiner <sup>1</sup> ; R. Farra <sup>1</sup> ; R. Schlögl <sup>1</sup> ; <sup>1</sup> Fritz Haber Institute of the Max Planck Society, Berlin/D
11:45	Thermal conductivity measurements on small samples – industrial relevance and applications M. Plass <sup>1</sup> ; C. Vo <sup>1</sup> ; <sup>1</sup> Dow Europe GmbH, Horgen/CH	About the influence of material morphology on photocatalytic hydrogen production T. Weller <sup>1</sup> ; M. Weiss <sup>1</sup> ; L. Specht <sup>1</sup> ; R. Marschall <sup>1</sup> ; <sup>1</sup> Justus-Liebig Universität Gießen/D
12:05	LUNCH BREAK	12:05

Friday, 26 May 2017

Afternoon

	Room: Audimax: 42-115	Chair
13:05	C.A.M. Seidel, Universität Düsseldorf/D <b>PLENARY LECTURE</b> Towards a Smallest Unit of Life P. Schwille; Max Planck Institute of Biochemistry, Martinsried/D	13:05
13:45	Quantum Control in Spectroscopy and Microscopy: Probing Biomolecules with Complex Laser Pulses M. Motzkus; Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg/D <b>PLENARY LECTURE</b>	13:45
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Award Session / Funding Symposium</b>
14:40	Molecular mechanisms of rheological behaviour in highly concentrated antibody solutions P. Garidel <sup>1</sup> ; J. Hartl <sup>2</sup> ; D. Johannsmann <sup>3</sup> ; <sup>1</sup> MLU Halle-Wittenberg, Biberach/D; <sup>2</sup> BI Pharma GmbH & Co KG, Biberach an der Riss/D; <sup>3</sup> Clausthal University of Technology, Clausthal-Zellerfeld/D	U. Nickel, HCS Goup, Frankfurt am Main/D <b>Ewald-Wicke Preis</b>
15:00	Linking Structure and Optical Spectra of Photosynthetic Antenna Complexes and Reaction Centers F. Mühl <sup>1</sup> ; M. Plöckinger <sup>1</sup> ; A. Gardiner <sup>2</sup> ; A. Roszak <sup>2</sup> ; R. Cogdell <sup>2</sup> ; J. Adolphs <sup>1</sup> ; T. Renger <sup>1</sup> ; <sup>1</sup> Johannes Kepler Universität Linz/A; <sup>2</sup> University of Glasgow/UK	Nernst-Haber-Bodenstein Preis
15:20	Thermophoresis and the 'Origin-of-Life' concept D. Niether <sup>1</sup> ; D. Afanasenkau <sup>1</sup> ; J. Dhont <sup>2</sup> ; S. Wiegand <sup>3</sup> ; <sup>1</sup> Forschungszentrum Jülich GmbH, Jülich/D; <sup>2</sup> Forschungszentrum Jülich GmbH, Heinrich-Heine-Universität Düsseldorf, Jülich/D; <sup>3</sup> Forschungszentrum Jülich GmbH, Universität zu Köln, Jülich/D	DFG Funding Opportunities for Early Career Researchers W. Wachter <sup>1</sup> ; J. Kowol-Santen <sup>1</sup> ; <sup>1</sup> Deutsche Forschungsgemeinschaft (DFG), Bonn/D
15:40	Time Resolved Light Scattering on Vimentin Aggregation in Dilute Aqueous Solution K. Huber <sup>1</sup> ; C. Lopez <sup>1</sup> ; O. Saldanha <sup>2</sup> ; S. Köster <sup>2</sup> ; <sup>1</sup> Universität Paderborn/D; <sup>2</sup> Universität Göttingen/D	
16:00	COFFEE BREAK	16:00
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Main Topic - Physical Chemistry for Life Sciences</b>
16:20	K. Blank, Max Planck Institute of Colloids and Interfaces, Potsdam/D <b>Investigation of Vibrational Energy Transfer in Various Biological Systems Using a Pair of Non-Canonical Amino Acids</b> K. Eberl <sup>1</sup> ; J. Löffler <sup>1</sup> ; P. Durkin <sup>2</sup> ; E. Deniz <sup>1</sup> ; D. Üresin <sup>1</sup> ; H. Müller-Werkmeister <sup>1</sup> ; T. Baumann <sup>2</sup> ; M. Hauf <sup>2</sup> ; F. Schildhauer <sup>2</sup> ; N. Budisa <sup>2</sup> ; J. Bredenbeck <sup>1</sup> ; <sup>1</sup> Goethe Universität Frankfurt/D; <sup>2</sup> Technische Universität Berlin/D	I. Bald, BAM-Bundesanstalt für Materialforschung und -prüfung, Berlin/D <b>Ultrafast photoinduced dynamics of a Ru(II) complex as model for photo active drugs</b> B. Dietzek <sup>1</sup> ; A. de la Cadena <sup>2</sup> ; <sup>1</sup> Friedrich-Schiller-University Jena/D; <sup>2</sup> Leibniz Institute of Photonic Technology, Jena/D
16:40	Spectroscopy of a promiscuous class of iron-sulfur cluster-containing dehydratases T. Pambe <sup>1</sup> ; M. Schneiderl <sup>1</sup> ; I. Kouker <sup>1</sup> ; H. Auerbach <sup>1</sup> ; C. Müller <sup>1</sup> ; V. Schünemann <sup>1</sup> ; A. Pierik <sup>2</sup> ; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> TU Kaiserslautern/Biochemie/D	<b>Computational Metallomics of the Anticancer Drug Cisplatin</b> V. Calandri <sup>1</sup> ; T. Nguyen <sup>2</sup> ; G. Rossetti <sup>3</sup> ; F. Arnesano <sup>4</sup> ; G. Natile <sup>4</sup> ; P. Carloni <sup>2</sup> ; <sup>1</sup> Forschungszentrum Jülich/D; <sup>2</sup> Computational Biomedicine IAS-5 and INM-9, Forschungszentrum Jülich/D; <sup>3</sup> Computational Biomedicine IAS-5 and INM-9, Jülich Supercomputing Centre (JSC) Forschungszentrum Jülich/D, and Department of Oncology, Hematology and Stem Cell Transplantation, RWTH Aachen University, Jülich/D; <sup>4</sup> Department of Chemistry, University of Bari/I
17:00	Conformational switches of a DnaB helicase during DNA replication studied by solid-state NMR T. Wiegand <sup>1</sup> ; K. Keller <sup>1</sup> ; D. Lacabanne <sup>2</sup> ; R. Cadalbert <sup>1</sup> ; L. Terradot <sup>2</sup> ; M. Yulikov <sup>1</sup> ; G. Jeschke <sup>1</sup> ; A. Böckmann <sup>2</sup> ; B. Meier <sup>1</sup> ; <sup>1</sup> ETH Zürich/CH; <sup>2</sup> CNRS/Université de Lyon/F	The Homochiral Serine Octamer: Infrared Spectrum and Structure of the Chloride Adduct G. von Helden <sup>1</sup> ; <sup>1</sup> Fritz Haber Institute of the Max Planck Society, Berlin/D
17:20	Probing the interplay between solvation dynamics and molecular-recognition in IDPS A. Chowdhury <sup>1</sup> ; I. Valle Aramburu <sup>1</sup> ; P. Tan <sup>1</sup> ; E. Lemke <sup>1</sup> ; <sup>1</sup> EMBL - European Molecular Biology Laboratory, Heidelberg/D	Correcting the record: The dimers and trimers of trans-N-methylacetamide T. Forsting <sup>1</sup> ; H. Gottschalk <sup>2</sup> ; B. Hartwig <sup>2</sup> ; M. Mons <sup>3</sup> ; M. Suhm <sup>2</sup> ; <sup>1</sup> Georg-August-Universität Göttingen/D; <sup>2</sup> Georg-August-Universität Göttingen, Institut für Physikalische Chemie/D; <sup>3</sup> LIDYL; CEA, CNRS, Université Paris-Saclay, Gif-sur-Yvette/F
17:40	Femtosecond Time-Resolved Ligand Dynamics in Myoglobin observed with an XFEL – Hunting for the Transition State H. Müller-Werkmeister <sup>1</sup> ; H. Ginn <sup>2</sup> ; A. Kuo <sup>3</sup> ; A. Sarracini <sup>3</sup> ; H. Duyvesteyn <sup>2</sup> ; S. Epp <sup>1</sup> ; D. Sherrell <sup>4</sup> ; D. Axford <sup>4</sup> ; S. Owada <sup>5</sup> ; O. Pare-Labrosse <sup>3</sup> ; S. Oghbaey <sup>3</sup> ; J. Besaw <sup>3</sup> ; Y. Kumagal <sup>6</sup> ; K. Tono <sup>5</sup> ; E. Schulz <sup>1</sup> ; P. Mehrabi <sup>3</sup> ; Y. Zhong <sup>1</sup> ; K. Motomura <sup>6</sup> ; B. Eger <sup>3</sup> ; A. Marx <sup>1</sup> ; E. Pai <sup>3</sup> ; A. Pearson <sup>7</sup> ; R. Owen <sup>4</sup> ; K. Ueda <sup>6</sup> ; D. Stuart <sup>8</sup> ; O. Ernst <sup>3</sup> ; R. Miller <sup>9</sup> ; <sup>1</sup> Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg/D; <sup>2</sup> University of Oxford/UK; <sup>3</sup> University of Toronto/CAN; <sup>4</sup> Diamond Light Source Ltd., Didcot/UK; <sup>5</sup> SACLA, RIKEN Spring-8 Center, Hyogo/J; <sup>6</sup> Tohoku University, Sendai/J; <sup>7</sup> Hamburg University & The Hamburg Center for Ultrafast Imaging/D; <sup>8</sup> University of Oxford & Diamond Light Source Ltd./UK; <sup>9</sup> Max-Planck-Institut für Struktur und Dynamik der Materie & University of Toronto, Hamburg/D	Lipid dependent insertion of the human N-BAR domain into 2D and 3D sarcolemma model membranes A. Auerswald <sup>1</sup> ; T. Gruber <sup>1</sup> ; G. Hause <sup>1</sup> ; J. Balbach <sup>1</sup> ; A. Meister <sup>1</sup> ; <sup>1</sup> Martin-Luther-Universität Halle-Wittenberg/D
	Room Mensa - Geb. 30	
18:15	POSTER SESSION (even numbers)	18:15
19:45	POSTER SESSION (odd numbers) (19:45-21:15)	19:45

## LECTURE PROGRAMME

Friday, 26 May 2017

Afternoon

	Room: Audimax: 42-115		
Chair	C.A.M. Seidel, Universität Düsseldorf/D	Chair	
13:05	<b>PLENARY LECTURE</b> Towards a Smallest Unit of Life <u>P. Schwille</u> ; Max Planck Institute of Biochemistry, Martinsried/D	13:05	
13:45	<b>PLENARY LECTURE</b> Quantum Control in Spectroscopy and Microscopy: Probing Biomolecules with Complex Laser Pulses <u>M. Motzkus</u> ; Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg/D	13:45	
	Room: HS 46-220	Room: HS 46-215	
	Surfaces and Interfaces	Solids and Nano-sized Matter	
Chair	B. Park, Universität Göttingen/D	N. Bigall, Universität Hannover/D	
14:40	<b>Atomic and Electronic Structure at Metal-Endofullerene / Metal Interfaces</b> <u>L. Kelly<sup>1</sup></u> ; J. Seidel <sup>1</sup> ; N. Haag <sup>1</sup> ; J. Stöckl <sup>1</sup> ; M. Franke <sup>2</sup> ; G. van Straaten <sup>2</sup> ; C. Kumpf <sup>2</sup> ; B. Stadtmüller <sup>1</sup> ; M. Cinchetti <sup>3</sup> ; M. Aeschlimann <sup>1</sup> ; <sup>1</sup> Department of Physics and Research Center OPTIMAS, University of Kaiserslautern/D; <sup>2</sup> Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich/D; <sup>3</sup> Experimentelle Physik VI, Technische Universität Dortmund/D	Probing Upconversion and Energy Transfer in Coupled Organic-Inorganic Nanostructures (COIN) by Transient Absorption Spectroscopy <u>J. Lauth<sup>1</sup></u> ; G. Grimaldi <sup>1</sup> ; S. Kinge <sup>2</sup> ; A. Houtepen <sup>1</sup> ; M. Scheele <sup>3</sup> ; L. Siebbeles <sup>1</sup> ; <sup>1</sup> Delft University of Technology, Delft/NL; <sup>2</sup> Toyota Motor Europe, Zaventem/B; <sup>3</sup> Universität Tübingen/D	14:40
15:00	<b>Spin-dependent dispersion of the hybrid band structure of the Alq3/Co interface</b> <u>J. Stöckl<sup>1</sup></u> ; A. Jurenkow <sup>1</sup> ; N. Großmann <sup>1</sup> ; B. Stadtmüller <sup>1</sup> ; M. Cinchetti <sup>2</sup> ; M. Aeschlimann <sup>1</sup> ; <sup>1</sup> TU Kaiserslautern/Department of Physics/D; <sup>2</sup> TU Dortmund/D	Optical Properties of Size-Selected Water-Soluble Ag-In-S and Core/Shell Ag-In-S/ZnS Quantum Dots <u>O. Stroyuk<sup>1</sup></u> ; A. Raevskaya <sup>1</sup> ; D. Haubold <sup>1</sup> ; V. Lesnyak <sup>1</sup> ; N. Gaponik <sup>1</sup> ; A. Eychmüller <sup>1</sup> ; V. Dzhagan <sup>2</sup> ; D. Zahn <sup>2</sup> ; <sup>1</sup> TU Dresden, Physikalische Chemie/D; <sup>2</sup> Semiconductor Physics, Chemnitz University of Technology/D	15:00
15:20	<b>Hoch spinselektive, metallisch/organische Grenzflächen am Beispiel des Modellsystems TCNE/Co(001)</b> <u>S. Lach<sup>1</sup></u> ; A. Altenhof <sup>1</sup> ; S. Shi <sup>2</sup> ; G. Lefkidis <sup>1</sup> ; M. Fahlman <sup>2</sup> ; C. Ziegler <sup>1</sup> ; <sup>1</sup> TU Kaiserslautern/Department of Physics/D; <sup>2</sup> Department of Physics, Chemistry and Biology (IFM), Linköping University/S	Protecting and Tuning of the Emission Properties of Highly Photoluminescent Nanocrystals <u>C. Guhrenz<sup>1</sup></u> ; A. Benad <sup>2</sup> ; C. Ziegler <sup>3</sup> ; C. Bauer <sup>2</sup> ; N. Gaponik <sup>2</sup> ; A. Eychmüller <sup>2</sup> ; <sup>1</sup> TU Dresden/D; <sup>2</sup> TU Dresden, Physikalische Chemie/D; <sup>3</sup> Nanyang Technological University, Singapore/SGP	15:20
15:40	<b>Selective Spin-Delivery by Metal-Complexes on Surfaces</b> <u>M. Prosenc<sup>1</sup></u> ; B. Bugenhagen <sup>2</sup> ; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Universität Hamburg/D	Nature and Stability of Paramagnetic Defects in Reducible Metal Oxide Nanoparticle Systems <u>M. Niedermayer<sup>1</sup></u> ; M. Schuhmann <sup>1</sup> ; K. Kocsis <sup>1</sup> ; T. Berger <sup>1</sup> ; O. Diwald <sup>1</sup> ; <sup>1</sup> University of Salzburg/A	15:40
16:00	COFFEE BREAK		16:00
	Theoretical Techniques	Experimental Techniques	
Chair	J. Paier, Humboldt-Universität zu Berlin/D	F. Merkt, ETH Zürich/CH	Chair
16:20	<b>Resolution of the identity employing Gaussian-type functions for solid state DFT and RPA methods</b> <u>A. Burow<sup>1</sup></u> ; <sup>1</sup> Ludwig-Maximilians University Munich/D	A study of excitation wavelength dependence of the effective fluorescence lifetime of toluene vapor <u>T. Endres<sup>1</sup></u> ; T. Benzler <sup>2</sup> ; T. Baranowski <sup>2</sup> ; T. Dreier <sup>2</sup> ; C. Schulz <sup>2</sup> ; <sup>1</sup> University of Duisburg-Essen, Duisburg/D; <sup>2</sup> Institute for Combustion and Gas Dynamics – Reactive Fluids, University of Duisburg-Essen, Duisburg/D	16:20
16:40	<b>Analytic Gradients for Complex-Valued Resonance Energies</b> <u>Z. Benda<sup>1</sup></u> ; <u>T. Jagau<sup>1</sup></u> ; <sup>1</sup> Ludwig-Maximilians-Universität München/D	BerlinTrap: A novel cryogenic 22-pole tandem mass spectrometer <u>P. Nieto<sup>1</sup></u> ; A. Günther <sup>1</sup> ; D. Müller <sup>1</sup> ; A. Sheldrick <sup>1</sup> ; <u>O. Dopfer<sup>1</sup></u> ; <sup>1</sup> TU Berlin/D	16:40
17:00	<b>On the Theoretical Optimization of Properties</b> <u>M. Springborg<sup>1</sup></u> ; <sup>1</sup> University of Saarland, Saarbrücken/D	Fourier Transform Microwave Spectroscopic Studies of Dimethyl Ether and Ethylene Flames <u>D. Obenchain<sup>1</sup></u> ; J. Wullenkord <sup>2</sup> ; K. Kohse-Höinghaus <sup>2</sup> ; J. Grabow <sup>3</sup> ; N. Hansen <sup>4</sup> ; <sup>1</sup> Gottfried Wilhelm Leibniz Universität Hannover/D; <sup>2</sup> Bielefeld University/D; <sup>3</sup> Gottfried Wilhelm Leibniz Universität Hannover/D; <sup>4</sup> Combustion Research Facility, Sandia National Laboratories, Livermore/CA/USA	17:00
17:20	<b>Quantum Mechanics in a Glass of Water</b> <u>T. Kühne<sup>1</sup></u> ; <sup>1</sup> University of Paderborn/D	Exploring the conformational dynamics of a DNA hairpin under the influence of osmolytes at both ambient and extreme environmental conditions <u>S. Patra<sup>1</sup></u> ; <sup>1</sup> TU Dortmund/D	17:20
17:40	<b>Theoretical studies on organometallic compounds from first principles using local CASPT2</b> <u>D. Kats<sup>1</sup></u> ; F. Menezes <sup>1</sup> ; H. Werner <sup>1</sup> ; <sup>1</sup> Universität Stuttgart/D	Maximizing the fluorescence signal and photostability of fluorophores by quenching dark states <u>D. Dörr<sup>1</sup></u> ; S. Kalinin <sup>2</sup> ; R. Kuehnemuth <sup>1</sup> ; D. Sandrin <sup>1</sup> ; O. Opanasyuk <sup>1</sup> ; D. Pfiffi <sup>3</sup> ; A. Chmyrov <sup>4</sup> ; B. Bier <sup>1</sup> ; T. Mueller <sup>1</sup> ; K. Schaper <sup>1</sup> ; J. Widengren <sup>5</sup> ; C. Seidel <sup>1</sup> ; <sup>1</sup> Heinrich-Heine-University Duesseldorf/D; <sup>2</sup> Carl Zeiss AG, Jena/D; <sup>3</sup> Roche Diagnostics GmbH, Mannheim/D; <sup>4</sup> Helmholtz Zentrum, München/D; <sup>5</sup> Royal Institute of Technology, Stockholm/S	17:40
	Room Mensa - Geb. 30		
18:15	POSTER SESSION (even numbers)		18:15
19:45	POSTER SESSION (odd numbers) (19:45-21:15)		19:45

Friday, 26 May 2017

Afternoon

	Room: Audimax: 42-115	
Chair	C.A.M. Seidel, Universität Düsseldorf/D	Chair
13:05	<b>PLENARY LECTURE</b> Towards a Smallest Unit of Life <u>P. Schwille</u> ; Max Planck Institute of Biochemistry, Martinsried/D	13:05
13:45	<b>PLENARY LECTURE</b> Quantum Control in Spectroscopy and Microscopy: Probing Biomolecules with Complex Laser Pulses <u>M. Motzkus</u> ; Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg/D	13:45
	Room: HS 46-210	Room: HS 46-110
	Molecular Structure	
Chair	D. Schooss, Karlsruhe Institute of Technology (KIT)/D	Chair
14:40	<b>Study of Intermolecular Interactions using Broadband Rotational Spectroscopy</b> M. Fatima <sup>1</sup> ; C. Perez <sup>1</sup> ; S. Zinn <sup>1</sup> ; M. Schnell <sup>1</sup> ; A. Poblotzki <sup>2</sup> ; M. Suhm <sup>2</sup> ; D. Bernhard <sup>3</sup> ; F. Dietrich <sup>3</sup> ; A. Stamm <sup>3</sup> ; M. Gerhards <sup>3</sup> ; <sup>1</sup> Max Planck Institute for Structure and Dynamics of Matter, Hamburg/D; <sup>2</sup> University of Göttingen/D; <sup>3</sup> TU Kaiserslautern/D	14:40
15:00	<b>IR/UV spectroscopic investigations on the diphenyl ether – tert-butyl alcohol complex in the electronic ground and excited state</b> D. Bernhard <sup>1</sup> ; F. Dietrich <sup>1</sup> ; A. Poblotzki <sup>2</sup> ; M. Fatima <sup>3</sup> ; C. Pérez <sup>3</sup> ; M. Suhm <sup>2</sup> ; M. Schnell <sup>3</sup> ; M. Gerhards <sup>1</sup> ; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Universität Göttingen/D; <sup>3</sup> Max Planck Institute for the Structure and Dynamics of Matter, Hamburg/D	15:00
15:20	<b>Water-Induced Zwitterionization of Glycine: Stabilization Mechanism and Spectral Signatures</b> <u>R. Pérez de Tudela</u> <sup>1</sup> ; D. Marx <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	15:20
15:40	<b>Small fragments of fullerenes: optical spectroscopy and astronomical relevance.</b> <u>D. Strelnikov</u> <sup>1</sup> ; M. Link <sup>1</sup> ; M. Kappes <sup>1</sup> ; <sup>1</sup> Institute of Physical Chemistry, KIT, Karlsruhe/D	15:40
16:00	COFFEE BREAK	16:00
	Molecular Structure	Electrochemistry and Energy
Chair	M. Suhm, Universität Göttingen/D	K.-M. Weitzel, Universität Marburg/D
16:20	<b>Hydrogen Induced Structure Change of Ruthenium Clusters</b> D. Bumüller <sup>1</sup> ; A. Hehn <sup>2</sup> ; E. Waldt <sup>1</sup> ; R. Ahlrichs <sup>2</sup> ; M. Kappes <sup>2</sup> ; <sup>1</sup> D. Schooss <sup>3</sup> ; <sup>1</sup> Karlsruhe Institute of Technology (KIT)/ Institute of Nanotechnology/D; <sup>2</sup> Karlsruhe Institute of Technology (KIT)/Institute of Physical Chemistry/D; <sup>3</sup> Karlsruhe Institute of Technology (KIT)/D	<b>Ultrafast Artificial Mixed Conductors</b> C. Chen <sup>1</sup> ; L. Fu <sup>1</sup> ; J. Maier <sup>1</sup> ; <sup>1</sup> Max Planck Institute for Solid State Research, Stuttgart/D
16:40	<b>Effect of Coordinated Radical Ligands on the Rate of Spin Crossover Processes in Iron(II) Complexes</b> <u>M. Schmitz</u> <sup>1</sup> ; H. Kelm <sup>1</sup> ; <u>H. Krüger</u> <sup>1</sup> ; <sup>1</sup> University of Kaiserslautern/D	An in-situ ATR-FTIR study of the electrochemical reduction of graphene oxide based on a novel electrode design M. Pfaffeneder-Kmen <sup>1</sup> ; G. Trettenhahn <sup>1</sup> ; W. Kautek <sup>1</sup> ; <sup>1</sup> University of Vienna/A
17:00	<b>Vibrational Spectroscopy of D2-Tagged Microhydrated Magnesium Nitrate Cations [MgNO3(H2O) 2-12] +</b> S. Debnath <sup>1</sup> ; X. Song <sup>2</sup> ; M. Fagiani <sup>2</sup> ; W. Schollkopf <sup>2</sup> ; S. Gewinner <sup>2</sup> ; L. Jiang <sup>3</sup> ; K. Asmis <sup>4</sup> ; <sup>1</sup> University of Leipzig/D; <sup>2</sup> Fritz Haber Institute of the Max Planck Society, Berlin/D; <sup>3</sup> Dalian Institute of Chemical Physics/CN; <sup>4</sup> University Leipzig/D	<b>High Voltage Aqueous Redox Flow Batteries Using Ionic Liquids</b> R. Chen <sup>1</sup> ; Z. Huang <sup>1</sup> ; Y. Zhang <sup>1</sup> ; R. Hempelmann <sup>1</sup> ; <sup>1</sup> Transfercentre Sustainable Electrochemistry, Saarland University, Saarbrücken/D
17:20	<b>Evidence for the presence and absence of clusters of like-charged ions in OH-functionalized ionic liquids</b> <u>T. Niemann</u> <sup>1</sup> ; A. Strate <sup>1</sup> ; R. Ludwig <sup>1</sup> ; <sup>1</sup> University of Rostock/ Institute of Chemistry, D	<b>Tuning of the Structure and Chemical Composition of the Nanoporous Copper for the CO<sub>2</sub> Reduction</b> M. Özaslan <sup>1</sup> ; B. Hecker <sup>1</sup> ; <sup>1</sup> Carl von Ossietzky Universität Oldenburg/D
17:40	<b>Interactions and Dynamics of Polyelectrolytes Mixed with Oppositely Charged Microemulsion Droplets</b> M. Simon <sup>1</sup> ; M. Gradzielski <sup>1</sup> ; <sup>1</sup> TU Berlin/D	<b>Modeling the migration energy in Zr/Y-codoped ceria</b> S. Grieshammer <sup>1</sup> ; <sup>1</sup> Forschungszentrum Jülich GmbH, Aachen/D
	Room Mensa - Geb. 30	
18:15	POSTER SESSION (even numbers)	18:15
19:45	POSTER SESSION (odd numbers) (19:45-21:15)	19:45

## LECTURE PROGRAMME

Saturday, 27 May 2017

Morning

	Room: Audimax: 42-115	
Chair	M. Gerhards, TU Kaiserslautern/D	Chair
08:30	<b>PLENARY LECTURE</b> New dimensions in biomolecular mass spectrometry and ion spectroscopy <u>T. Rizzo</u> <sup>1</sup> ; <sup>1</sup> EPFL, Lausanne/CH	08:30
	Room: Audimax: 42-115	Room: HS 42-110
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Main Topic - Physical Chemistry for Life Sciences</b>
Chair	J. Heberle, Freie Universität Berlin/D	G. Niedner-Schatteburg, TU Kaiserslautern/D
09:25	<b>An in depth study of replica-based molecular dynamics methods for protein conformational sampling</b> <u>D. Möller</u> <sup>1</sup> ; M. Kulke <sup>1</sup> ; N. Geist <sup>1</sup> ; W. Langel <sup>1</sup> ; <sup>1</sup> Universität Greifswald/D	<b>Conformations of protonated noradrenaline and its alkali metal complexes studied by an electrospray and a cold ion trap laser spectroscopy</b> <u>M. Fujii</u> <sup>1</sup> ; <sup>1</sup> Tokyo Institute of Technology, Yokohama/J
09:45	<b>Folding Stability of a RNA Hairpin – The Role of Hydration, Osmolytes, and Crowding</b> <u>M. Gao</u> <sup>1</sup> ; L. Arns <sup>1</sup> ; D. Gnutt <sup>2</sup> ; S. Ebbinghaus <sup>2</sup> ; R. Winter <sup>1</sup> ; <sup>1</sup> TU Dortmund/D; <sup>2</sup> Ruhr-Universität Bochum/D	<b>Optical photodissociation spectroscopy of metal-lumichrome ionic complexes using the 22-pole BerlinTrap</b> <u>D. Müller</u> <sup>1</sup> ; <u>P. Nieto</u> <sup>1</sup> ; A. Günther <sup>1</sup> ; A. Sheldrick <sup>1</sup> ; O. Dopfer <sup>1</sup> ; <sup>1</sup> TU Berlin/D
10:05	<b>Solvatochromism of nitriles to probe local protein dynamics</b> <u>L. van Wilderen</u> <sup>1</sup> ; H. Brunst <sup>1</sup> ; J. Bredenbeck <sup>1</sup> ; <sup>1</sup> Goethe Universität Frankfurt/D	<b>Laser-desorption conformer-specific IR spectroscopy of sulfonamide drugs: Tautomeric and conformational preferences, and intermolecular interactions of the sulfonamide group</b> <u>T. Uhlemann</u> <sup>1</sup> ; S. Seidel <sup>1</sup> ; <u>C. Müller</u> <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D
10:25	<b>Cosolute effects on protein folding stability</b> <u>S. Ebbinghaus</u> <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	<b>Computational solvation dynamics of oxyquinolinium betaine linked to various disaccharides</b> <u>E. Heid</u> <sup>1</sup> ; A. Szabadi <sup>1</sup> ; C. Schröder <sup>1</sup> ; <sup>1</sup> Faculty of Chemistry, University of Vienna/A
10:45	COFFEE BREAK	
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Main Topic - Physical Chemistry for Life Sciences</b>
Chair	R. Diller, TU Kaiserslautern/D	S. Keller, TU Kaiserslautern/D
11:05	<b>Full Lecture</b> <b>The Grateful Infrared – Novel IR techniques to probe the functional changes of membrane proteins</b> <u>J. Heberle</u> <sup>1</sup> ; <sup>1</sup> Freie Universität Berlin/D	<b>Tissue-based Cancer Diagnostics with Surface-Enhanced Raman Spectroscopy and Imaging</b> <u>S. Schlücker</u> <sup>1</sup> ; <u>M. König</u> <sup>1</sup> ; Y. Zhang <sup>1</sup> ; X. Wang <sup>1</sup> ; <sup>1</sup> Universität Duisburg-Essen, Fakultät für Chemie, Essen/D
11:25		<b>Penetration mechanisms of Core-multishell (CMS) nanocarrier in human and mouse skin studied by Stimulated Raman spectromicroscopy</b> <u>A. Klossek</u> <sup>1</sup> ; K. Yamamoto <sup>2</sup> ; K. Yamamoto <sup>2</sup> ; S. Höinzke <sup>2</sup> ; H. Pischon <sup>2</sup> ; M. Radbruch <sup>2</sup> ; L. Mundhenk <sup>2</sup> ; A. Gruber <sup>2</sup> ; S. Hedtrich <sup>2</sup> ; E. Rühl <sup>2</sup> ; <sup>1</sup> Freie Universität Berlin, Institut für Chemie und Biochemie, Physikalische und Theoretische Chemie, D; <sup>2</sup> Freie Universität Berlin/D
11:45	<b>Membrane-Solubilizing Properties of Amphiphilic Copolymers</b> <u>A. Grethen</u> <sup>1</sup> ; R. Cuevas Arenas <sup>1</sup> ; A. Oluwole <sup>1</sup> ; C. Vargas <sup>1</sup> ; S. Keller <sup>1</sup> ; <sup>1</sup> University of Kaiserslautern/D	<b>DNA origami based substrates for surface-enhanced Raman scattering (SERS)</b> <u>I. Bald</u> <sup>1</sup> ; J. Prinz <sup>1</sup> ; C. Heck <sup>1</sup> ; <sup>1</sup> University of Potsdam, Germany/D
12:05	<b>Imidazolium salts imitating the structure of lipids reveal remarkable properties forming lamellar phases, giant vesicles and fluidizing bilayer membranes</b> <u>P. Dräger</u> <sup>1</sup> ; A. Rühling <sup>2</sup> ; D. Grill <sup>3</sup> ; D. Wang <sup>4</sup> ; A. Draeger <sup>1</sup> ; V. Gerke <sup>3</sup> ; F. Glorius <sup>2</sup> ; H. Galla <sup>4</sup> ; <sup>1</sup> Universität Bern/ Institut für Anatomie/CH; <sup>2</sup> Westfälische Wilhelms-Universität Münster/ Organisch-Chemisches Institut/D; <sup>3</sup> Westfälische Wilhelms-Universität Münster/ ZMBE/D; <sup>4</sup> Westfälische Wilhelms-Universität Münster/ Institut für Biochemie/D	<b>Spot variation fluorescence correlation spectroscopy without spot variation – easy way to study living cells</b> <u>S. Jebreil Khadem</u> <sup>1</sup> ; C. Hille <sup>2</sup> ; H. Löhmansröben <sup>3</sup> ; I. Sokolov <sup>4</sup> ; <sup>1</sup> Humboldt-Universität zu Berlin, D; <sup>2</sup> University of Potsdam, Institute of Chemistry/D; <sup>3</sup> University of Potsdam, Institute of Chemistry/D; <sup>4</sup> Humboldt University Berlin, Institute of Physics/D
12:25	LUNCH BREAK	

Saturday, 27 May 2017

Morning

	Room: Audimax: 42-115	
Chair	M. Gerhards, TU Kaiserslautern/D	Chair
08:30	<b>PLENARY LECTURE</b> New dimensions in biomolecular mass spectrometry and ion spectroscopy <u>T. Rizzo</u> <sup>1</sup> ; <sup>1</sup> EPFL, Lausanne/CH	08:30
	Room: HS 46-220	Room: HS 46-215
	<b>Liquids and Solvation</b>	<b>Solids and Nano-sized Matter</b>
Chair	R. Ludwig, Universität Rostock/D	J. Lauth, TU Delft/NL
09:25	<b>The H-bond dynamics of aqueous solutions under high pressure</b> <u>H. Vondracek</u> <sup>1</sup> ; L. Knake <sup>1</sup> ; I. Kolling <sup>1</sup> ; G. Schwaab <sup>1</sup> ; M. Havenith <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	<b>Size, Shape and Phase Control in Ultrathin CdSe Nanosheets</b> <u>C. Klinke</u> <sup>1</sup> ; <sup>1</sup> University of Hamburg/D
09:45	<b>Supra-additive slowdown of water rotation by outer-sphere ion pairs</b> A. Vila Verde <sup>1</sup> ; R. Lipowsky <sup>1</sup> ; <sup>1</sup> MPI für Kolloid- und Grenzflächenforschung, Potsdam/D	<b>Controlling Heterogeneous Nucleation and Particle Shape in Hybrid Nanoparticle Synthesis</b> D. Hinrichs <sup>1</sup> ; A. Wolf <sup>1</sup> ; <u>D. Dorfs</u> <sup>1</sup> ; <sup>1</sup> Leibniz Universität Hannover/D
10:05	<b>On the complex structural diffusion of the solvated hydroxide in nanoconfined water</b> <u>D. Muñoz-Santiburcio</u> <sup>1</sup> ; D. Marx <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	<b>Electrostatic Shielding versus Sterical Ligand Stabilization: Tunable Nanocrystal Stabilization Mechanisms</b> <u>L. Mohrhüsen</u> <sup>1</sup> ; M. Osmic <sup>1</sup> ; J. Kolny-Olesiak <sup>1</sup> ; K. Al-Shamery <sup>1</sup> ; <sup>1</sup> University of Oldenburg/D
10:25	<b>Hydration dynamics in CaCO<sub>3</sub> nucleation by THz spectroscopy</b> <u>F. Sebastiani</u> <sup>1</sup> ; S. Wolf <sup>2</sup> ; B. Born <sup>1</sup> ; T. Luong <sup>3</sup> ; H. Cölfen <sup>2</sup> ; D. Gebauer <sup>2</sup> ; M. Havenith <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D; <sup>2</sup> University of Konstanz/D	<b>Multifunctional MOF nanoparticles via self-assembly</b> U. Lächelt <sup>1</sup> ; R. Röder <sup>1</sup> ; P. Hirschle <sup>2</sup> ; T. Preiß <sup>3</sup> ; A. Zimpel <sup>2</sup> ; J. Rädler <sup>3</sup> ; E. Wagner <sup>1</sup> ; T. Bein <sup>2</sup> ; <u>S. Wuttke</u> <sup>4</sup> ; <sup>1</sup> LMU München, Pharmazie/D; <sup>2</sup> Fakultät für Chemie und Pharmazie, LMU München/D; <sup>3</sup> LMU München, Physik/D; <sup>4</sup> LMU München/D
10:45	COFFEE BREAK	
	<b>Liquids and Solvation</b>	<b>Catalysis</b>
Chair	F. Sebastiani, Ruhr-Universität Bochum/D	J.P. Hofmann, TU Eindhoven/NL
11:05	<b>Structure and dynamics of clusters of like-charged ions in ionic liquids</b> A. Strate <sup>1</sup> ; T. Niemann <sup>1</sup> ; V. Lehde <sup>1</sup> ; R. Ludwig <sup>1</sup> ; <sup>1</sup> University of Rostock/D	<b>LEED-I(V) Analysis of the (7x3)rect Structure on the Ag(111) Surface</b> R. Wyrwich <sup>1</sup> ; T. Jones <sup>2</sup> ; W. Moritz <sup>1</sup> ; S. Günther <sup>3</sup> ; M. Ehrensperger <sup>1</sup> ; S. Böcklein <sup>1</sup> ; T. Mentes <sup>4</sup> ; A. Locatelli <sup>4</sup> ; M. Nino <sup>4</sup> ; S. Piccinin <sup>5</sup> ; A. Knop-Gericke <sup>2</sup> ; R. Schlögl <sup>2</sup> ; <u>J. Winterlin</u> <sup>1</sup> ; <sup>1</sup> Ludwig-Maximilians-Universität München (LMU)/D; <sup>2</sup> Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D; <sup>3</sup> Technische Universität München/D; <sup>4</sup> SINTEF Trondheim, Trondheim/N; <sup>5</sup> CNR-IOM Democritos Trieste/I
11:25	<b>Mixtures of Ionic Liquids and Alcohols studied by Computer Simulations</b> <u>D. Kerlé</u> <sup>1</sup> ; <sup>1</sup> Universität Bremen/D	<b>New insights in Au activation mechanism in CO oxidation.</b> A. Klyushin <sup>1</sup> ; E. Carbonio <sup>2</sup> ; T. Jones <sup>3</sup> ; M. Hävecker <sup>3</sup> ; E. Frei <sup>3</sup> ; M. Lamoth <sup>3</sup> ; E. Willinger <sup>3</sup> ; A. Knop-Gericke <sup>4</sup> ; R. Schlögl <sup>3</sup> ; <sup>1</sup> Helmholtz-Zentrum Berlin/D; <sup>2</sup> Helmholtz-Zentrum Berlin für Materialien und Energie/D; <sup>3</sup> Fritz-Haber-Institute of the Max Planck Society, Berlin/D
11:45	<b>Critical and Non-critical Mesoscopic Inhomogeneities in Solutions of the Protic Ionic Liquids Ethyl-Ammonium Nitrate and n-Alkyl Alcohols</b> O. Russina <sup>1</sup> ; A. Triolo <sup>2</sup> ; W. Schröer <sup>3</sup> ; <u>B. Rathke</u> <sup>4</sup> ; <sup>1</sup> Dipartimento di Chimica, Università di Roma Sapienza/I; <sup>2</sup> Istituto Struttura della Materia, Consiglio Nazionale delle Ricerche, Rome/I; <sup>3</sup> Institut für Anorganische und Physikalische Chemie, Universität Bremen/D; <sup>4</sup> Technische Thermodynamik, Universität Bremen/D	<b>Time-resolved IR spectroscopic studies of Sr-NaTaO<sub>3</sub> photocatalysts</b> <u>X. Yu</u> <sup>1</sup> ; C. Yang <sup>1</sup> ; S. Heissler <sup>1</sup> ; A. Nefedov <sup>1</sup> ; H. Onishi <sup>2</sup> ; Y. Wang <sup>1</sup> ; C. Wöll <sup>1</sup> ; <sup>1</sup> Karlsruhe Institute of Technology (KIT)/Institute of Functional Interfaces, Eggenstein-Leopoldshafen/D; <sup>2</sup> Kobe University/School of Science/Department of Chemistry, Nada, Kobe/J
12:05	<b>Structure, Dynamics and Mixing Energies in Protic Ionic Liquids. Influence of Anions and Cations: A Molecular Dynamics Simulation Study</b> <u>B. Golub</u> <sup>1</sup> ; D. Paschek <sup>1</sup> ; R. Ludwig <sup>1</sup> ; <sup>1</sup> University of Rostock/Institute of Chemistry/D	<b>Activation of O<sub>2</sub> on nanoporous gold revisited: associative versus dissociative mechanism</b> L. Moskaleva <sup>1</sup> ; M. Bäumer <sup>1</sup> ; W. Dononelli <sup>2</sup> ; T. Klüner <sup>2</sup> ; <sup>1</sup> Universität Bremen, D; <sup>2</sup> Carl von Ossietzky Universität Oldenburg/D
12:25	LUNCH BREAK	

## LECTURE PROGRAMME

Saturday, 27 May 2017

Morning

	Room: Audimax: 42-115	
Chair	M. Gerhards, TU Kaiserslautern/D	Chair
08:30	<b>PLENARY LECTURE</b> New dimensions in biomolecular mass spectrometry and ion spectroscopy <u>T. Rizzo</u> <sup>1</sup> ; <sup>1</sup> EPFL, Lausanne/CH	08:30
	Room: HS 46-210	Room: HS 46-110
	Chemical Dynamics and Kinetics	Electrochemistry and Energy
Chair	C. Riehn, TU Kaiserslautern/D	R. Marschall, Universität Giessen/D
09:25	<b>New Insights into the Photodissociation of Bisphenyl(2,4,6 trimethylbenzoyl)phosphine oxide</b> S. Straub <sup>1</sup> ; C. Lohrmann <sup>1</sup> ; J. Lindner <sup>1</sup> ; P. Vöhringer <sup>1</sup> ; <sup>1</sup> Rheinische Friedrich-Wilhelms-Universität Bonn/D	Ultrafast carrier dynamics of the perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ on mesoporous titania scaffolds in contact with hole transport materials J. Klein <sup>1</sup> ; J. Hölzer <sup>1</sup> ; M. Scholz <sup>1</sup> ; K. Oum <sup>1</sup> ; <u>T. Lenzer</u> <sup>1</sup> ; <sup>1</sup> Universität Siegen, Physikalische Chemie/D
09:45	<b>Photophysical Properties of Phthalimides</b> A. Reiffers <sup>1</sup> ; C. Torres <sup>1</sup> ; P. Gilch <sup>1</sup> ; <sup>1</sup> Heinrich-Heine-Universität Düsseldorf/D	Nature and Relevance of ion conduction and charge transport in $\text{CH}_3\text{NH}_3\text{PbI}_3$ G. Kim <sup>1</sup> ; A. Senocrate <sup>1</sup> ; I. Moudrakovski <sup>1</sup> ; T. Yang <sup>1</sup> ; G. Gregori <sup>1</sup> ; M. Grätzel <sup>2</sup> ; J. Maier <sup>1</sup> ; <sup>1</sup> Max Planck Institute for Solid State Research, Stuttgart/D; <sup>2</sup> Department of Chemistry and Chemical Engineering, Swiss Federal Institute of Technology (EPFL), Lausanne/CH
10:05	<b>Sensitivity of the Ultrafast Deactivation of Berenil to the Biomolecular Binding Partner</b> L. Grimmelsmann <sup>1</sup> ; C. Spies <sup>1</sup> ; J. Knorr <sup>1</sup> ; <u>P. Nuernberger</u> <sup>1</sup> ; <sup>1</sup> Ruhr-Universität Bochum/D	Electrocatalysis with Atomically-Defined Model Systems Prepared and Characterized in Ultrahigh Vacuum Conditions: CO Electro-Oxidation on Pt/Co3O4(111) O. Brummel <sup>1</sup> ; C. Stumm <sup>1</sup> ; M. Bertram <sup>1</sup> ; F. Faisal <sup>1</sup> ; S. Cherevko <sup>2</sup> ; K. Mayrhofer <sup>2</sup> ; F. Xiang <sup>1</sup> ; M. Schneider <sup>1</sup> ; J. Libuda <sup>1</sup> ; <sup>1</sup> FAU Erlangen-Nürnberg/D; <sup>2</sup> Jülich GmbH, Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy (IEK-11)/D
10:25	<b>The primary photochemical processes upon laser flash photolysis of a puckered ferrocyclobutadiene in liquid solution studied by ultrafast femtosecond mid-infrared spectroscopy</b> B. Weiszla <sup>1</sup> ; J. Lindner <sup>1</sup> ; <u>P. Vöhringer</u> <sup>1</sup> ; <sup>1</sup> Rheinische Friedrich-Wilhelms-Universität Bonn/D	Shape-engineering of metallic aerogels for electrocatalysis <u>B. Cai</u> <sup>1</sup> ; A. Eychmüller <sup>1</sup> ; <sup>1</sup> TU Dresden/D
10:45	COFFEE BREAK	
	Chemical Dynamics and Kinetics	Surfaces and Interfaces
Chair	S. Landgraf, TU Graz/A	K. Boldt, Universität Konstanz/D
11:05	<b>Experimental studies of the ion-molecule reactions <math>\text{H}^{2+} + \text{H}_2</math> and <math>\text{H}^{2+} + \text{D}_2</math> at low collision energies in a merged beam apparatus</b> K. Höveler <sup>1</sup> ; P. Allmendinger <sup>1</sup> ; J. Deiglmayr <sup>1</sup> ; O. Schullian <sup>1</sup> ; F. Merkt <sup>1</sup> ; <sup>1</sup> ETH Zürich/CH	Molecular Topology and Metal/Organic Interfaces B. Klein <sup>1</sup> ; N. van der Heijden <sup>2</sup> ; C. Krug <sup>1</sup> ; M. Schöniger <sup>1</sup> ; P. Rosenow <sup>1</sup> ; M. Schmid <sup>1</sup> ; R. Tonner <sup>1</sup> ; I. Swart <sup>2</sup> ; J. Gottfried <sup>1</sup> ; <sup>1</sup> Philipps-Universität Marburg/D; <sup>2</sup> Debye Institute for Nanomaterial Science, Utrecht University/NL
11:25	<b>Imaging the reaction dynamics the base-induced elimination</b> E. Carrascosa <sup>1</sup> ; J. Meyer <sup>1</sup> ; J. Zhang <sup>2</sup> ; M. Stein <sup>1</sup> ; T. Michaelsen <sup>1</sup> ; L. Yang <sup>2</sup> ; W. Hase <sup>3</sup> ; R. Wester <sup>1</sup> ; <sup>1</sup> Institute für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck/A; <sup>2</sup> School of Chemistry and Chemical Engineering, Harbin Institute of Technology/CN; <sup>3</sup> Department of Chemistry and Biochemistry, Texas Tech University, Lubbock/USA	Synthesis and surface characterization of hydrothermal carbon materials and their application in water electrolysis S. Buller <sup>1</sup> ; P. Düngen <sup>1</sup> ; J. Straten <sup>1</sup> ; Y. Yi <sup>2</sup> ; F. Wachholz <sup>1</sup> ; R. Schlögl <sup>1</sup> ; <sup>1</sup> Max-Planck-Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D; <sup>2</sup> Max-Planck-Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D
11:45	<b>Ultrafast and angle-resolved photoelectron spectroscopy of multiply charged anions</b> M. Winghart <sup>1</sup> ; A. Veenstra <sup>1</sup> ; J. Yang <sup>1</sup> ; A. Unterreiner <sup>1</sup> ; M. Kappes <sup>1</sup> ; <sup>1</sup> Karlsruher Institut für Technologie (KIT)/D	Examination of Buried Interfaces Between Transition Metal Layers and Tetrapyrrole Films with Hard X-ray Photoelectron Spectroscopy M. Schmid <sup>1</sup> ; M. Chen <sup>1</sup> ; M. Zugermeier <sup>1</sup> ; B. Klein <sup>1</sup> ; C. Krug <sup>1</sup> ; S. Kachel <sup>1</sup> ; J. Gottfried <sup>1</sup> ; <sup>1</sup> Philipps-Universität Marburg/D
12:05	<b>Chemistry and Photochemistry of Hydrated Metal Ions in the Gas Phase: Lessons Learned from <math>\text{Mg}^+</math> and <math>\text{Al}^+</math></b> M. Ončák <sup>1</sup> ; T. Taxer <sup>1</sup> ; C. van der Linde <sup>1</sup> ; M. Beyer <sup>1</sup> ; <sup>1</sup> Universität Innsbruck/A	Photoelectron Angular Distributions of Free Silica Nanoparticles as a Probe for Photoelectron Scattering Processes E. Antonsson <sup>1</sup> ; B. Langer <sup>1</sup> ; I. Halfpap <sup>1</sup> ; J. Gottwald <sup>1</sup> ; E. Rühl <sup>1</sup> ; <sup>1</sup> Freie Universität Berlin/D
12:25	LUNCH BREAK	

**Saturday, 27 May 2017****Afternoon**

	Room: Audimax: 42-115	
Chair	J. Küpper, Universität Hamburg/D	Chair
13:30	<b>PLENARY LECTURE</b> <b>Forces and Conformational Dynamics in Biomolecular Nanomachines</b> H. Grubmüller <sup>1</sup> ; L. Bock <sup>1</sup> ; A. Vaiana <sup>1</sup> ; <sup>1</sup> Max Planck Institute for Biophysical Chemistry, Göttingen/D	13:30
	Room: Audimax: 42-115	Room: HS 42-110
	<b>Main Topic - Physical Chemistry for Life Sciences</b>	<b>Main Topic - Physical Chemistry for Life Sciences</b>
Chair	T. Gutmann, TU Darmstadt/D	S. Ebbinghaus, Ruhr-Universität Bochum/D
14:25	<b>Lipid-coated Iron Metal-Organic Framework Nanoparticles for Biomedical Applications</b> B. Illes <sup>1</sup> ; A. Zimpel <sup>1</sup> ; P. Hirschle <sup>1</sup> ; S. Krombholz <sup>1</sup> ; S. Wuttke <sup>1</sup> ; H. Engelke <sup>1</sup> ; <sup>1</sup> LMU München/D	Key difference between type I and type II cryptochromes and implication for their role in magnetoreception R. Kutta <sup>1</sup> ; N. Archipowa <sup>2</sup> ; L. Johannissen <sup>2</sup> ; A. Jones <sup>1</sup> ; N. Scrutton <sup>2</sup> ; <sup>1</sup> Manchester Institute of Biotechnology (MIB) and School of Chemistry, The University of Manchester/UK and Photon Science Institute (PSI) and School of Chemistry, The University of Manchester/UK; <sup>2</sup> Manchester Institute of Biotechnology (MIB) and School of Chemistry, The University of Manchester/UK
14:45	<b>Sub-molecular Structure and Orientation of Oligonucleotide Duplexes Tethered to Gold Electrodes Probed by Infrared Reflection Absorption Spectroscopy: Effect of the Electrode Potentials</b> L. Kekedy-Nagy <sup>1</sup> ; E. Ferapontova <sup>1</sup> ; I. Brand <sup>2</sup> ; <sup>1</sup> Aarhus University, Aarhus/DK; <sup>2</sup> University of Oldenburg/D	<b>Shining Light on Nature's Raincoat: Infrared Insights on Hydrophobins</b> K. Meister <sup>1</sup> ; A. Paaninen <sup>2</sup> ; H. Bakker <sup>1</sup> ; <sup>1</sup> FOM Institute AMOLF, Amsterdam/D; <sup>2</sup> VTT Research Centre of Finland, Tampere/FIN
15:05	<b>Detection of biomolecules with fiber-optical sensing by using fiber-Bragg-gratings</b> S. Schulze <sup>1</sup> ; M. Wehrhold <sup>1</sup> ; C. Hille <sup>1</sup> ; <sup>1</sup> University of Potsdam, Institute of Chemistry / Physical Chemistry, Potsdam OT Golm/D	<b>Analysis of an Unusually Long-Lived Tyrosyl Radical by Time-resolved IR and UV/vis Spectroscopy</b> S. Oldemeyer <sup>1</sup> ; S. Franz <sup>2</sup> ; S. Wenzel <sup>3</sup> ; L. Essen <sup>2</sup> ; M. Mittag <sup>3</sup> ; T. Kottke <sup>1</sup> ; <sup>1</sup> Bielefeld University/D; <sup>2</sup> Philipps University Marburg/D; <sup>3</sup> Friedrich Schiller University Jena/D
15:25	<b>Solubilization of Membrane Proteins into Functional Lipid-Bilayer Nanodiscs by Diisobutylene/Maleic Acid Copolymer</b> A. Oluwole <sup>1</sup> ; B. Danielczak <sup>1</sup> ; A. Meister <sup>2</sup> ; J. Babalola <sup>1</sup> ; C. Vargas <sup>1</sup> ; S. Keller <sup>1</sup> ; <sup>1</sup> University of Kaiserslautern/D; <sup>2</sup> Martin Luther University Halle-Wittenberg/D	<b>Enzyme Adsorption-induced Activity Changes: A Quantitative Study on TiO<sub>2</sub> Model Agglomerates</b> A. Márquez <sup>1</sup> ; T. Berger <sup>1</sup> ; A. Feinle <sup>1</sup> ; N. Hüsing <sup>1</sup> ; M. Himly <sup>1</sup> ; A. Duschl <sup>1</sup> ; O. Diwald <sup>1</sup> ; <sup>1</sup> Universität Salzburg/A
	Room: Audimax: 42-115	
16:00	<b>Poster Awards and Closing Session</b>	16:00

## LECTURE PROGRAMME

**Saturday, 27 May 2017****Afternoon**

	Room: Audimax: 42-115	
Chair	J. Küpper, Universität Hamburg/D	Chair
13:30	<b>PLENARY LECTURE</b> <b>Forces and Conformational Dynamics in Biomolecular Nanomachines</b> H. Grubmüller <sup>1</sup> ; L. Bock <sup>1</sup> ; A. Vaiana <sup>1</sup> ; <sup>1</sup> Max Planck Institute for Biophysical Chemistry, Göttingen/D	13:30
	Room: HS 46-220	Room: HS 46-215
	<b>Liquids and Solvation</b>	<b>Catalysis</b>
Chair	A. Vila Verde, MPI für Kolloid- und Grenzflächenforschung, Potsdam/D	J. Wintterlin, Ludwig-Maximilians Universität München/D
14:25	<b>Femtosecond spectroscopy of the solvated electron in liquid ammonia over a wide range of excitation energies</b> T. Vogler <sup>1</sup> ; J. Lindner <sup>2</sup> ; P. Vöhringer <sup>2</sup> ; <sup>1</sup> Universität Bonn/D; <sup>2</sup> Institut für Physikalische und Theoretische Chemie, Universität Bonn/D	<b>Gas Phase Modeling of the Catalytically Active Centers in Iron Sulfur Proteins</b> H. Heim <sup>1</sup> ; T. Bernhardt <sup>1</sup> ; S. Lang <sup>2</sup> ; <sup>1</sup> Universität Ulm, Institut für Oberflächenchemie und Katalyse/D; <sup>2</sup> Universität Ulm/D
14:45	<b>Investigation of Diffusion Processes by Solvatochromism in a Microfluidic Setup</b> H. Fischer <sup>1</sup> ; M. Muth <sup>1</sup> ; E. Antonsson <sup>1</sup> ; E. Rühl <sup>1</sup> ; <sup>1</sup> Freie Universität Berlin/D	<b>Ligands on Nanoparticles – Combining the Benefits of Homogeneous and Heterogeneous Catalysis</b> I. Schrader <sup>1</sup> ; S. Neumann <sup>1</sup> ; A. Sulce <sup>1</sup> ; S. Kunz <sup>1</sup> ; <sup>1</sup> Institute of Applied and Physical Chemistry (IAPC), University of Bremen/D
15:05	<b>Calculation of Two-Particle Entropies in Bulk Fluids and Solutions</b> D. Huggins <sup>1</sup> ; B. Irwin <sup>1</sup> ; <sup>1</sup> University of Cambridge/UK	<b>Fundamental studies on photocatalytic CO<sub>2</sub> reduction</b> M. Dilla <sup>1</sup> ; S. Ristig <sup>2</sup> ; J. Strunk <sup>3</sup> ; <sup>1</sup> Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr/D; <sup>2</sup> Max-Planck-Institut für chemische Energiekonversion, Mülheim an der Ruhr/D; <sup>3</sup> Leibniz-Institut für Katalyse, Rostock/D
15:25	<b>An Experimental Test of Fermi's Golden Rule using Femtosecond IR Pump-Probe Spectroscopy</b> J. Gleim <sup>1</sup> ; T. Unruh <sup>1</sup> ; D. Czurlok <sup>1</sup> ; J. Lindner <sup>1</sup> ; P. Vöhringer <sup>1</sup> ; <sup>1</sup> Institut für Physikalische und Theoretische Chemie, Universität Bonn/D	<b>Understanding Reaction Mechanisms in Heterogeneously Catalyzed Reactions: The Case of Catalytic Fast Pyrolysis</b> P. Hemberger <sup>1</sup> ; <sup>1</sup> Paul Scherrer Institut (PSI), Villigen PSI/CH
	Room: Audimax: 42-115	
16:00	<b>Poster Awards and Closing Session</b>	16:00

**Saturday, 27 May 2017****Afternoon**

	Room: Audimax: 42-115	
Chair	<i>J. Küpper, Universität Hamburg/D</i>	Chair
13:30	<b>PLENARY LECTURE</b> <b>Forces and Conformational Dynamics in Biomolecular Nanomachines</b> <u>H. Grubmüller</u> <sup>1</sup> ; L. Bock <sup>1</sup> ; A. Vaiana <sup>1</sup> ; <sup>1</sup> Max Planck Institute for Biophysical Chemistry, Göttingen/D	13:30
	Room: HS 46-210	Room: HS 46-110
	Chemical Dynamics and Kinetics	Hot Topic
Chair	<i>P. Nürnberg, Ruhr-Universität Bochum/D</i>	<i>D. Horke, Center for Free-Electron Laser Science, DESY and The Hamburg Centre for Ultrafast Imaging, Hamburg/D</i>
14:25	<b>Excited State Dynamics of Photoactive Copper(I) Complexes with an Extended <math>\pi</math>-System</b> M. Karnahl <sup>1</sup> ; S. Lochbrunner <sup>2</sup> ; <u>S. Tschierle</u> <sup>3</sup> ; <sup>1</sup> Universität Stuttgart/D; <sup>2</sup> Universität Rostock/D; <sup>3</sup> Universität Ulm/D	<b>Inferring the gas-phase structure of lanthanoid complexes with biologically relevant ligands by combining gas-phase photoluminescence, action, and ion mobility spectroscopies with quantum chemical computations</b> J. Greisch <sup>1</sup> ; M. Harding <sup>1</sup> ; J. Chmelář <sup>1</sup> ; J. Lang <sup>2</sup> ; G. Niedner-Schatteburg <sup>2</sup> ; W. Klopper <sup>1</sup> ; D. Schooss <sup>1</sup> ; M. Kappes <sup>1</sup> ; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; <sup>2</sup> Technische Universität Kaiserslautern/D
14:45	<b>Electron and hole transfer processes of triarylamine solar cell dyes bound to mesoporous TiO<sub>2</sub>, ZnO and Al<sub>2</sub>O<sub>3</sub> thin films studied by femtosecond UV-Vis-NIR spectroscopy</b> M. Scholz <sup>1</sup> ; O. Flender <sup>1</sup> ; <u>K. Oum</u> <sup>2</sup> ; T. Lenzer <sup>1</sup> ; <sup>1</sup> Universität Siegen, Physikalische Chemie/D; <sup>2</sup> Universität Siegen/D	<b>Bulk diffusion versus grain-boundary diffusion of potassium through praseodymium-manganese oxide</b> J. Martin <sup>1</sup> ; T. Kramer <sup>2</sup> ; C. Jooss <sup>3</sup> ; <u>K. Weitzer</u> <sup>3</sup> ; <sup>1</sup> Fachbereich Chemie, Philipps-Universität Marburg, Germany, D; <sup>2</sup> Georg-August-Universität Göttingen/D; <sup>3</sup> Philipps-Universität Marburg/D
15:05	<b>Individual Tuning of Solvent Properties – Introduction and Application to Ionic Liquids</b> <u>S. Landgraf</u> <sup>1</sup> ; M. Berghold <sup>1</sup> ; J. Bächle <sup>1</sup> ; <sup>1</sup> TU Graz/A	<b>Towards a Femtosecond Resolved View of the Mechanisms of the Hydrogen Evolution Reaction on Au</b> Y. Tong <sup>1</sup> ; F. Lapointe <sup>1</sup> ; <u>R. Campen</u> <sup>1</sup> ; <sup>1</sup> Fritz Haber Institute of the Max Planck Society, Berlin/D
15:25	<b>Ultrafast dynamics of a Ni-porphyrin based magnetically bistable molecular switch by fs transient absorption spectroscopy</b> <u>S. Megow</u> <sup>1</sup> ; <sup>1</sup> Christian-Albrechts-Universität zu Kiel/D	<b>Imaging nanoscale morphology of semiconducting polymer films with photoemission electron microscopy</b> F. Niefeld <sup>1</sup> ; A. Neff <sup>1</sup> ; B. Abel <sup>1</sup> ; M. Hamsch <sup>2</sup> ; S. Mannsfeld <sup>2</sup> ; K. Siefermann <sup>1</sup> ; <sup>1</sup> Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig/D; <sup>2</sup> Center for Advancing Electronics Dresden/D
	Room: Audimax: 42-115	
16:00	<b>Poster Awards and Closing Session</b>	16:00

## POSTER PROGRAMME

## Main Topic – Physical Chemistry for Life Sciences

- P 01.01 **Plasmonic Nanosensors for the Determination of Drug Effectiveness on Membrane Receptors**  
R. Ahijado-Guzmán<sup>1</sup>; C. Sönnichsen<sup>1</sup>; <sup>1</sup> JGU-Mainz/D
- P 01.02 **Multiplexed targeting of cells and tissue – novel surface-modulated upconversion nanoparticles for biosensing and -imaging**  
S. Nacak<sup>1</sup>; P. Bastian<sup>1</sup>; M. Kumke<sup>1</sup>; <sup>1</sup> Universität Potsdam/Physikalische Chemie /D
- P 01.03 **Electron-induced single and double strand breaks in DNA determined by using the DNA origami technique**  
K. Ebel<sup>1</sup>; <sup>1</sup> University of Potsdam, Institute of Chemistry/ Physical Chemistry/D
- P 01.04 **The photochemical mechanism of a B12-dependent photoreceptor protein**  
R. Kutta<sup>1</sup>; S. Hardman<sup>2</sup>; L. Johannissen<sup>3</sup>; B. Bellina<sup>4</sup>; H. Messiha<sup>3</sup>; J. Ortiz-Guerrero<sup>5</sup>; M. Elías-Arnanz<sup>6</sup>; S. Padmanabhan<sup>7</sup>; P. Barran<sup>4</sup>; N. Scrutton<sup>3</sup>; A. Jones<sup>8</sup>; <sup>1</sup> Manchester Institute of Biotechnology (MIB) and School of Chemistry, The University of Manchester/UK and Photon Science Institute (PSI) and School of Chemistry, The University of Manchester/UK, Manchester/UK; <sup>2</sup> SYNBIOCHEM, Manchester Institute of Biotechnology, The University of Manchester/UK. and Faculty of Life Sciences, The University of Manchester/UK; <sup>3</sup> SYNBIOCHEM, Manchester Institute of Biotechnology, The University of Manchester, UK and Faculty of Life Sciences, The University of Manchester/UK; <sup>4</sup> School of Chemistry, The University of Manchester/UK and SYNBIOCHEM, Manchester Institute of Biotechnology, The University of Manchester/UK; <sup>5</sup> Department of Genetics and Microbiology, Universidad de Murcia/E; <sup>6</sup> Department of Genetics and Microbiology, Universidad de Murcia/E; <sup>7</sup> Instituto de Química Física 'Rocasolano', Consejo Superior de Investigaciones Científicas, Spain, Madrid/E; <sup>8</sup> School of Chemistry, The University of Manchester/UK, Photon Science Institute (PSI), The University of Manchester/UK, and SYNBIOCHEM, Manchester Institute of Biotechnology, The University of Manchester/UK
- P 01.05 **Photoinduced processes of free bilins in solution studied by fs TA absorption spectroscopy**  
M. Theiß<sup>1</sup>; T. Lamarter<sup>2</sup>; M. Mroginski<sup>3</sup>; R. Diller<sup>1</sup>; <sup>1</sup> TU Kaiserslautern, Abt. Biophysik /D; <sup>2</sup> KIT, Karlsruhe/D; <sup>3</sup> TU Berlin /D
- P 01.06 **Spectral Signature of Cooperative H-Bonding in Gas Phase Cyanide-Water Clusters**  
J. Kelly<sup>1</sup>; H. Knorke<sup>2</sup>; J. Barnes<sup>1</sup>; K. Asmis<sup>1</sup>; <sup>1</sup> Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig/D; <sup>2</sup> Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Leipzig University/D
- P 01.07 **Chiral effects and changes in hydrophobicity due to CH<sub>3</sub>>CF<sub>3</sub> mutations in proteins**  
J. Robalo<sup>1</sup>; S. Huhmann<sup>2</sup>; B. Koksch<sup>2</sup>; A. Vila Verde<sup>1</sup>; <sup>1</sup> MPI für Kolloid- und Grenzflächenforschung, Potsdam/D; <sup>2</sup> Freie Universität Berlin/D
- P 01.08 **Thermophoresis of cyclodextrins and cyclodextrin-drug-complexes**  
D. Niether<sup>1</sup>; K. Eguchi<sup>2</sup>; T. Kawaguchi<sup>2</sup>; J. Hovancová<sup>3</sup>; R. Kita<sup>2</sup>; S. Wiegand<sup>4</sup>; <sup>1</sup> Forschungszentrum Jülich GmbH/D; <sup>2</sup> Tokai University, Hiratsuka/J; <sup>3</sup> Pavol Jozef Safarik University, Kosice/SK; <sup>4</sup> Forschungszentrum Jülich GmbH, Universität zu Köln/D
- P 01.09 **Studying the Solvation Dynamics of Model Peptides in Water via Fourier Transform Terahertz/Far-Infrared Absorption Spectroscopy**  
C. Ma<sup>1</sup>; G. Schwaab<sup>1</sup>; M. Havenith<sup>1</sup>; <sup>1</sup> Ruhr University Bochum/D
- P 01.10 **Multidimensional infrared studies of cyanylated cysteins in a photosensor protein**  
J. Schmidt-Engler<sup>1</sup>; L. Blankenburg<sup>2</sup>; F. Habenstein<sup>2</sup>; L. van Wilderen<sup>2</sup>; J. Bredenbeck<sup>2</sup>; <sup>1</sup> Goethe-Universität Frankfurt am Main/D; <sup>2</sup> Goethe University Frankfurt, Institute of Biophysics/D
- P 01.11 **Following the photo-induced structure changes and dynamics of the photoreceptor PYP with an IR label**  
L. Blankenburg<sup>1</sup>; F. Habenstein<sup>1</sup>; L. Schröder<sup>2</sup>; T. Kottke<sup>2</sup>; J. Bredenbeck<sup>1</sup>; <sup>1</sup> Goethe University Frankfurt, Institute of Biophysics/D; <sup>2</sup> University Bielefeld, Physical and Biophysical Chemistry/D
- P 01.12 **Assembly of proteins and oriented purple membrane on functionalized carbon nanomembranes**  
N. Frese<sup>1</sup>; D. Rhinow<sup>2</sup>; A. Turchanin<sup>3</sup>; R. Riedel<sup>4</sup>; N. Hampp<sup>4</sup>; A. Götzhäuser<sup>1</sup>; <sup>1</sup> Bielefeld University/D; <sup>2</sup> Max Planck Institute of Biophysics, Frankfurt/D; <sup>3</sup> Friedrich Schiller University Jena/D; <sup>4</sup> Philipps University Marburg/D
- P 01.13 **Analyzing the Biocatalytic Halogenation of Tryptophan via the Photoreduction of Flavin**  
L. Schröder<sup>1</sup>; N. Sewald<sup>2</sup>; T. Kottke<sup>2</sup>; <sup>1</sup> Universität Bielefeld/D; <sup>2</sup> Bielefeld University/D

- P 01.14 **Exploring the early signaling mechanism of a short light-oxygen-voltage photoreceptor from Rhodobacter sphaeroides**  
I. Stambolic<sup>1</sup>; B. Dick<sup>1</sup>; <sup>1</sup> University of Regensburg/D
- P 01.15 **The short light-, oxygen-, voltage-sensitive domain from R. sphaeroides is a rapidly exchanging dimer in the dark**  
K. Magerl<sup>1</sup>; B. Dick<sup>1</sup>; <sup>1</sup> University of Regensburg/D
- P 01.16 **Membrane fusion trajectories derived from AFM force-clamp experiments**  
H. Witt<sup>1</sup>; M. Oelkers<sup>1</sup>; P. Halder<sup>2</sup>; R. Jahn<sup>2</sup>; A. Janshoff<sup>1</sup>; <sup>1</sup> Georg-August-Universität Göttingen/D; <sup>2</sup> Max Planck Institute for Biophysical Chemistry, Göttingen/D
- P 01.17 **Radiosensitization of DNA towards low energy electrons with 8-Bromoadenine**  
R. Schürmann<sup>1</sup>; I. Bald<sup>1</sup>; <sup>1</sup> Universität Potsdam/Physikalische Chemie/D
- P 01.18 **Secondary structure of fusion peptides anchored in non-lamellar membranes of monoolein**  
A. Levin<sup>1</sup>; C. Jeworrek<sup>1</sup>; R. Winter<sup>1</sup>; C. Czeslik<sup>1</sup>; <sup>1</sup> TU Dortmund/D
- P 01.19 **Surfactants influence the surface affinity of ions**  
S. Das<sup>1</sup>; <sup>1</sup> Max Planck Institute for Polymer Research, Mainz/D
- P 01.20 **Revisiting the photochemistry of the light-dependent NADPH:protochlorophyllide oxidoreductase**  
N. Archipowa<sup>1</sup>; R. Kutta<sup>1</sup>; N. Scrutton<sup>1</sup>; <sup>1</sup> Manchester Institute of Biotechnology (MIB) and School of Chemistry, The University of Manchester/UK
- P 01.21 **Endothelial cells studies by vibrational spectroscopy**  
M. Baranska<sup>1</sup>; <sup>1</sup> Jagiellonian University, Krakow/PL
- P 01.22 **Near infrared detection of cellular communication using fluorescent nanosensors**  
D. Meyer<sup>1</sup>; E. Polo<sup>1</sup>; A. Hagemann<sup>2</sup>; S. Kruss<sup>1</sup>; <sup>1</sup> Universität Göttingen/D; <sup>2</sup> Georg-August-Universität Göttingen/D
- P 01.23 **Energies of Solvation and Osmotic Coefficients in Mixtures of Tetraethylammonium Serinate with Water, Cytosolic Water or Calcic Cytosolic Water.**  
G. Ahn-Ercan<sup>1</sup>; <sup>1</sup> ComputeChem/ Universität Regensburg, Saal an der Donau/D
- P 01.24 **Sequence-specific ionization potentials of oligonucleotides correlated with VUV-induced DNA strand breaks**  
S. Vogel<sup>1</sup>; A. Milosavljevic<sup>2</sup>; A. Giuliani<sup>2</sup>; I. Bald<sup>1</sup>; <sup>1</sup> University of Potsdam/D; <sup>2</sup> Synchrotron SOLEIL, Gif-sur-Yvette/F
- P 01.25 **SPECTROSCOPIC STUDY OF UPCONVERTING STRONTIUM FLUORIDE NANOCRYSTALS PREPARED VIA SOL GEL SYNTHESIS**  
M. Monks<sup>1</sup>; <sup>1</sup> BAM Federal Institute for Material Research and Testing, Berlin/D
- P 01.26 **Combined IR/UV investigations on isolated peptides: structural assignments for cyclic tetrapeptides**  
D. Mauel<sup>1</sup>; A. Stamm<sup>1</sup>; K. Schwing<sup>1</sup>; A. Schaly<sup>1</sup>; S. Schlicher<sup>1</sup>; J. Bartl<sup>1</sup>; S. Kubik<sup>1</sup>; M. Gerhards<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D
- P 01.27 **Surface-enhanced Raman spectroscopy in life science**  
D. Cialla-May<sup>1</sup>; K. Weber<sup>1</sup>; J. Popp<sup>1</sup>; <sup>1</sup> Leibniz-Institut für Photonische Technologien, Jena/D
- P 01.28 **How to choose the optimal uncaging system for the VIPER pulse sequence**  
D. Kern-Michler<sup>1</sup>; C. Neumann<sup>1</sup>; L. van Wilderen<sup>1</sup>; M. Reinfelds<sup>1</sup>; A. Heckel<sup>1</sup>; J. Bredenbeck<sup>1</sup>; <sup>1</sup> Universität Frankfurt/D
- P 01.29 **Exploring the properties of hydroxylated coenzyme Q and its analogues**  
E. Slowik<sup>1</sup>; K. Stankoska<sup>1</sup>; N. Mitreska<sup>1</sup>; K. Reindl<sup>1</sup>; R. Gulaboski<sup>2</sup>; V. Mirceski<sup>3</sup>; M. Hoth<sup>1</sup>; I. Bogeski<sup>1</sup>; R. Kappl<sup>1</sup>; <sup>1</sup> Universität des Saarlandes/Biophysik, Homburg/D; <sup>2</sup> Universitiy Goce Delcev/Chemistry, Stip/MK; <sup>3</sup> University „SS Cyril and Methodius“/Chemistry, Skopje/MK

## POSTER PROGRAMME

- P 01.30 **Spin probing EPR-spectroscopic study of protein-protein interactions of a monoclonal antibody in highly concentrated solutions**  
V. Núñez<sup>1</sup>; J. Blaffert<sup>1</sup>; P. Garidel<sup>2</sup>; D. Hinderberger<sup>1</sup>; <sup>1</sup> Martin-Luther-Universität Halle-Wittenberg/D; <sup>2</sup> Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riß/D
- P 01.31 **Characterisation of a novel [2Fe-2S] cluster type via chemogenomic and EPR based studies**  
C. Blinn<sup>1</sup>; K. Stegmaier<sup>1</sup>; D. Bechtel<sup>1</sup>; A. Pierik<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/ Biochemie/D
- P 01.32 **Investigation of the structural heterogeneity in the cyanobacteriochrome AnPixJg2 by mutagenesis**  
P. Ahlert<sup>1</sup>; L. Scarbath-Evers<sup>1</sup>; S. Jähnigen<sup>1</sup>; S. Altmayer<sup>2</sup>; C. Song<sup>2</sup>; J. Matysik<sup>2</sup>; D. Sebastiani<sup>1</sup>; <sup>1</sup> Martin-Luther-Universität Halle-Wittenberg/D; <sup>2</sup> Universität Leipzig/D
- P 01.33 **Surface-Enhanced Raman Spectroscopy-Based Optical Nanosensor for CO Sensing in Living Cells**  
X. Zheng<sup>1</sup>; G. Reddy<sup>2</sup>; U. Neugebauer<sup>3</sup>; D. Cialla-May<sup>4</sup>; K. Weber<sup>4</sup>; A. Schiller<sup>2</sup>; J. Popp<sup>4</sup>; <sup>1</sup> Leibniz Institute of Photonic Technology, Jena/D; <sup>2</sup> Institute for Inorganic and Analytical Chemistry, Friedrich Schiller University Jena/D; <sup>3</sup> Leibniz Institute of Photonic Technology; Center for Sepsis Control and Care, Jena University Hospital; Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena/D; <sup>4</sup> Leibniz Institute of Photonic Technology; Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena/D
- P 01.34 **Application of Confocal Raman Microscopy in Cryobiology**  
A. Kreiner<sup>1</sup>; F. Stracke<sup>1</sup>; H. Zimmermann<sup>1</sup>; <sup>1</sup> Fraunhofer IBMT, Sulzbach/D
- P 01.35 **Protein-ligand thermodynamics from combining explicit simulation with integral equation-based approaches**  
Y. Alber<sup>1</sup>; F. Mrugalla<sup>1</sup>; S. Kast<sup>1</sup>; <sup>1</sup> TU Dortmund, Fakultät für Chemie und Chemische Biologie/D
- P 01.36 **pH-dependent tautomeric and conformational equilibria of the neurotransmitter histamine in aqueous solution**  
L. Eberlein<sup>1</sup>; J. Heil<sup>1</sup>; W. Hiller<sup>1</sup>; P. Schummel<sup>1</sup>; R. Winter<sup>1</sup>; S. Kast<sup>1</sup>; <sup>1</sup> TU Dortmund, Fakultät für Chemie und Chemische Biologie/D
- P 01.37 **Photoexcitation induced water reorientation dynamics in the 5-hydroxyindole-water cluster studied by time resolved IR spectroscopy**  
M. Miyazaki<sup>1</sup>; A. Naito<sup>1</sup>; J. Klyne<sup>2</sup>; O. Dopfer<sup>2</sup>; M. Fujii<sup>1</sup>; <sup>1</sup> Tokyo Institute of Technology, Yokohama/J; <sup>2</sup> TU Berlin/D
- P 01.38 **Optimal EC-RISM quantum solvation models for physicochemical characterization of drug-like molecules**  
N. Tielker<sup>1</sup>; D. Tomazic<sup>1</sup>; J. Heil<sup>1</sup>; T. Kloss<sup>2</sup>; S. Ehrhart<sup>3</sup>; S. Güssregen<sup>4</sup>; F. Schmidt<sup>4</sup>; S. Kast<sup>1</sup>; <sup>1</sup> TU Dortmund, Fakultät für Chemie und Chemische Biologie/D; <sup>2</sup> CEA, INAC, Grenoble/F; <sup>3</sup> CERN, Geneva/CH; <sup>4</sup> Sanofi-Aventis Deutschland GmbH, Frankfurt am Main/D
- P 01.39 **Photodissociation spectroscopy of protonated leucine enkephalin**  
A. Herburger<sup>1</sup>; C. van der Linde<sup>1</sup>; M. Beyer<sup>1</sup>; <sup>1</sup> Universität Innsbruck/A
- P 01.40 **Ionic selectivity of hydrophobic nanopores with physiological relevance**  
M. Urban<sup>1</sup>; L. Henkes<sup>1</sup>; S. Kast<sup>1</sup>; <sup>1</sup> TU Dortmund, Fakultät für Chemie und Chemische Biologie/D
- P 01.42 **Synthesis and Characterization of Small Gold Nanorods for Cellular Uptake by Neutrophil Granulocytes**  
M. Erkelenz<sup>1</sup>; J. Hee-Yoon<sup>1</sup>; E. Stepula<sup>1</sup>; V. Tran<sup>1</sup>; M. König<sup>1</sup>; R. Grzeschik<sup>1</sup>; K. Bruderek<sup>1</sup>; S. Brandau<sup>1</sup>; S. Schlücker<sup>1</sup>; <sup>1</sup> Universität Duisburg-Essen/D
- P 01.43 **Vibrational Energy Transfer in Tryptophan Zippers**  
J. Löffler<sup>1</sup>; K. Eberl<sup>1</sup>; E. Deniz<sup>1</sup>; P. Durkin<sup>2</sup>; N. Budisa<sup>2</sup>; J. Bredenbeck<sup>1</sup>; <sup>1</sup> Goethe Universität Frankfurt, Institut für Biophysik/D; <sup>2</sup> Technische Universität Berlin, Institut für Chemie/D
- P 01.44 **EPR spectroscopy of histidine-coordinated Iron-Sulfur Clusters**  
D. Bechtel<sup>1</sup>; K. Stegmaier<sup>1</sup>; A. Pierik<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/ Biochemie/D
- P 01.45 **Analysis of Light-Induced Protein Reactions in Intact Cells Using FTIR and Fluorescence Spectroscopy**  
J. Klocke<sup>1</sup>; T. Kottke<sup>1</sup>; <sup>1</sup> Bielefeld University/D

- P 01.46 **Evaluation of EPR spectroscopy and MST for the analysis of protein-protein interactions at high protein concentrations**  
J. Blaffert<sup>1</sup>; P. Garidel<sup>2</sup>; D. Hinderberger<sup>1</sup>; <sup>1</sup> Martin-Luther-Universität Halle-Wittenberg/D; <sup>2</sup> Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riß/D
- P 01.47 **High Resolution X-Ray Microscopy: Investigating Drug and Nanoparticle Penetration in Skin and Reconstructed Human Skin**  
K. Yamamoto<sup>1</sup>; A. Klossek<sup>1</sup>; R. Flesch<sup>1</sup>; F. Rancan<sup>2</sup>; M. Giulbudagian<sup>1</sup>; T. Ohigashi<sup>3</sup>; M. Weigand<sup>4</sup>; I. Bykova<sup>4</sup>; M. Bechtel<sup>4</sup>; P. Patoka<sup>1</sup>; G. Ulrich<sup>1</sup>; S. Ahlberg<sup>2</sup>; A. Vogt<sup>2</sup>; U. Blume-Peytavi<sup>2</sup>; P. Schrade<sup>5</sup>; S. Bachmann<sup>5</sup>; M. Calderón<sup>1</sup>; M. Schäfer-Korting<sup>6</sup>; R. Haag<sup>1</sup>; N. Kosugi<sup>3</sup>; E. Rühl<sup>1</sup>; <sup>1</sup> Institut für Chemie und Biochemie, Freie Universität Berlin/D; <sup>2</sup> Klinisches Forschungszentrum für Haut- und Haarforschung, Charité Universitätsklinikum, Berlin/D; <sup>3</sup> UVSOR Facility, Institute for Molecular Science, Okazaki/J; <sup>4</sup> Max-Planck-Institute for Intelligent Systems, Stuttgart/D; <sup>5</sup> Abteilung für Elektronenmikroskopie at CVK, Berlin/D; <sup>6</sup> Institut für Pharmazie, Freie Universität Berlin/D
- P 01.48 **Photoswitching diarylethene derivatives studied by absorption spectroscopy on a femto- and picosecond time scale**  
C. Schweigert<sup>1</sup>; O. Babii<sup>2</sup>; S. Afonin<sup>3</sup>; I. Komarov<sup>4</sup>; A. Ulrich<sup>5</sup>; A. Unterreiner<sup>6</sup>; <sup>1</sup> Karlsruhe Institute of Technology (KIT), Institute of Physical Chemistry/D; <sup>2</sup> KIT, Institute of Organic Chemistry/D; <sup>3</sup> KIT, Institute of Biological Interfaces (IBG-2)/D; <sup>4</sup> Shevchenko National University of Kyiv, Institute of High Technologies/UA; <sup>5</sup> KIT, Institute of Organic Chemistry and Institute of Biological Interfaces (IBG-2)/D; <sup>6</sup> KIT, Molecular Physical Chemistry, Institute of Physical Chemistry/D
- P 01.49 **Investigation of the Targeted Delivery and Biological Application of Biofunctionalized Gold Nanoparticles**  
L. Prisner<sup>1</sup>; N. Bohn<sup>2</sup>; P. Witthöft<sup>2</sup>; L. Nguyen<sup>2</sup>; T. Gefken<sup>2</sup>; T. Tsangas<sup>2</sup>; A. Mews<sup>2</sup>; <sup>1</sup> Universität Hamburg/D; <sup>2</sup> University of Hamburg, Institute of Physical Chemistry/D
- P 01.50 **Outside-In and Inside-Out activation mechanism of Integrin αVβ3**  
M. Kulke<sup>1</sup>; W. Langel<sup>1</sup>; <sup>1</sup> Universität Greifswald/D
- P 01.51 **STED-MFIS microscopy: Studying biomolecular systems beyond the diffraction limit with molecular resolution**  
J. Budde<sup>1</sup>; C. Seidel<sup>1</sup>; <sup>1</sup> Heinrich Heine University, Molekulare Physikalische Chemie, Düsseldorf/D
- P 01.52 **Characterizing and Optimizing a Novel Laser Desorption Source**  
N. Teschmit<sup>1</sup>; D. Horke<sup>1</sup>; K. Długoł cki<sup>2</sup>; D. Gusa<sup>2</sup>; I. Rubinsky<sup>2</sup>; J. Küpper<sup>3</sup>; <sup>1</sup> Center for Free-Electron Laser Science, DESY and The Hamburg Centre for Ultrafast Imaging/D; <sup>2</sup> Center for Free-Electron Laser Science, DESY, Hamburg/D; <sup>3</sup> Center for Free-Electron Laser Science, DESY, The Hamburg Centre for Ultrafast Imaging and Universität Hamburg/D
- P 01.53 **Model-Free Identification of Demixing in Binary Fluorocarbon/Hydrocarbon Surfactant Mixtures**  
E. Frotscher<sup>1</sup>; J. Höring<sup>1</sup>; G. Durand<sup>2</sup>; C. Vargas<sup>1</sup>; S. Keller<sup>1</sup>; <sup>1</sup> University of Kaiserslautern/D; <sup>2</sup> University of Avignon/F
- P 01.54 **Influence of Lipid Bilayer Properties on Nanodisc Formation**  
C. Vargas<sup>1</sup>; R. Cuevas Arenas<sup>1</sup>; J. Klingler<sup>1</sup>; S. Keller<sup>1</sup>; <sup>1</sup> University of Kaiserslautern/D
- P 01.55 **Raman microscopy for detection and enumeration of tumor cells**  
R. Kiselev<sup>1</sup>; C. Krafft<sup>2</sup>; J. Popp<sup>2</sup>; <sup>1</sup> Leibniz Institute of Photonic Technology, Jena/D; <sup>2</sup> Leibniz Institute for Photonic Technology, Jena/D
- P 01.56 **Distinguishing Isomeric Oligosaccharides Using Cold Ion Infrared Spectroscopy for Glycan Fingerprinting**  
E. Mucha<sup>1</sup>; A. González Flórez<sup>1</sup>; M. Marianski<sup>1</sup>; D. Thomas<sup>1</sup>; S. Gewinner<sup>1</sup>; S. Wieland<sup>1</sup>; P. Seeberger<sup>2</sup>; G. von Helden<sup>1</sup>; K. Pagel<sup>3</sup>; <sup>1</sup> Fritz Haber Institute of the Max Planck Society, Berlin/D; <sup>2</sup> Max Planck Institute of Colloids and Interfaces, Potsdam/D; <sup>3</sup> Freie Universität Berlin/D
- P 01.57 **Modeling the Intramolecular Interactions that initiate secretion of an Autotransporter protein**  
H. Mouhib<sup>1</sup>; T. Verzijden<sup>2</sup>; S. Abeln<sup>2</sup>; P. van Ulzen<sup>2</sup>; G. Wuite<sup>2</sup>; <sup>1</sup> Université Paris-Est Marne-La-Vallée/F; <sup>2</sup> VU Amsterdam/NL


**POSTER PROGRAMME**

- P 01.58 **Modulation of the Polymerization Kinetics of  $\alpha/\beta$ -Tubulin by Osmolytes and Macromolecular Crowding**  
P. Schummel<sup>1</sup>; M. Gao<sup>1</sup>; R. Winter<sup>1</sup>; <sup>1</sup> TU Dortmund/D
- P 01.59 **Pressure-induced Effects on Self-cleavage Catalysis of Ribozymes: A Molecular Dynamics Study**  
N. Kumar<sup>1</sup>; D. Marx<sup>1</sup>; <sup>1</sup> Ruhr-Universität Bochum/D
- P 01.60 **Electronic and vibrational properties of the NO heme interactions of Nitrophorin 2**  
H. Auerbach<sup>1</sup>; I. Faus<sup>1</sup>; S. Rackwitz<sup>1</sup>; J. Wolny<sup>1</sup>; F. Walker<sup>2</sup>; A. Chumakov<sup>3</sup>; V. Schünemann<sup>1</sup>; <sup>1</sup> University of Kaiserslautern/D; <sup>2</sup> The University of Arizona, Tucson/USA; <sup>3</sup> European Synchrotron Radiation Facility, Grenoble/F
- P 01.61 **Simulations of hyperfine parameters of dimetal-carboxylate-cofactor proteins**  
J. Marx<sup>1</sup>; R. Kositzki<sup>2</sup>; J. Griese<sup>3</sup>; V. Srinivas<sup>3</sup>; P. Schrapers<sup>2</sup>; M. Haumann<sup>2</sup>; M. Högbom<sup>3</sup>; V. Schünemann<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Free University of Berlin/D; <sup>3</sup> Stockholm University/S
- P 01.62 **DFT calculations for structural analysis of iron-sulfur clusters - impact of model and cluster environment**  
C. Müller<sup>1</sup>; H. Auerbach<sup>1</sup>; J. Marx<sup>1</sup>; J. Wolny<sup>1</sup>; V. Schünemann<sup>1</sup>; <sup>1</sup> University of Kaiserslautern/D
- P 01.63 **Hofmeister Effects in aqueous Oligopeptide solutions: The Termini matter for Guanidinium salts**  
V. Balos<sup>1</sup>; M. Bonn<sup>1</sup>; J. Hunger<sup>1</sup>; <sup>1</sup> Max Planck Institute for Polymer Research, Mainz/D
- P 01.64 **Impact of the Three Dimensional Nanostructure on the Determination of Diffusion Characteristics within Cell Membranes**  
P. Hagemann<sup>1</sup>; A. Gesper<sup>1</sup>; P. Happel<sup>1</sup>; <sup>1</sup> Ruhr University Bochum/D
- P 01.65 **Influence of Backbone Hydrogen Bonding on the Stability of the WW domain of the Protein Pin1**  
D. Markthaler<sup>1</sup>; <sup>1</sup> Universität Stuttgart/D
- P 01.66 **Quantifying the thermodynamic cost of protein desolvation**  
M. Heyden<sup>1</sup>; <sup>1</sup> Max-Planck-Institut für Kohlenforschung / Cluster of Excellence RESOLV, Mülheim an der Ruhr/D
- P 01.67 **Solid supported and soft cushioned biomimetic model membranes for investigation of transport processes through membranes**  
I. Kiesel<sup>1</sup>; Y. Gerelli<sup>2</sup>; G. Fragneto<sup>2</sup>; <sup>1</sup> TU Dortmund/D; <sup>2</sup> Institut Laue Langevin, Grenoble/D

### Liquids and Solvation

- P 02.01 **A Molecular Dynamics Simulation Study of Like-Charged Hydrogen Bonding in Ionic Liquids**  
J. Neumann<sup>1</sup>; D. Paschek<sup>2</sup>; R. Ludwig<sup>2</sup>; <sup>1</sup> Universität Rostock/D; <sup>2</sup> Universität Rostock, Institut für Chemie/D
- P 02.02 **THz Resonances of Water Molecules around Hydrophilic and Hydrophobic Groups of Trimethylamine N-oxide**  
S. Imoto<sup>1</sup>; H. Forbert<sup>2</sup>; D. Marx<sup>2</sup>; <sup>1</sup> Ruhr-Universität Bochum/D; <sup>2</sup> Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum/D
- P 02.03 **Second Osmotic Virial Coefficient for Polar and Nonpolar Solutes in Aqueous Solution from Molecular Simulation**  
E. Reiter<sup>1</sup>; <sup>1</sup> Universität Rostock/D
- P 02.04 **Local curvature determines water dynamics near small hydrophobic molecules but not near hydrophobic protein sites**  
J. Robalo<sup>1</sup>; A. Vila Verde<sup>1</sup>; <sup>1</sup> MPI für Kolloid- und Grenzflächenforschung, Potsdam/D
- P 02.05 **Non-Gaussian displacement distributions in aqueous electrolyte solutions**  
A. Vila Verde<sup>1</sup>; <sup>1</sup> MPI für Kolloid- und Grenzflächenforschung, Potsdam/D
- P 02.06 **Solute-solvent interactions and dynamics probed by THz light**  
G. Schwaab<sup>1</sup>; F. Böhm<sup>1</sup>; C. Ma<sup>1</sup>; F. Sebastiani<sup>1</sup>; M. Havenith<sup>1</sup>; <sup>1</sup> Ruhr-Universität Bochum/D

- P 02.07 **THz Spectroscopy of the Model Peptide N-Acetyl-Leucine Amide**  
H. Wirtz<sup>1</sup>; S. Schäfer<sup>2</sup>; A. Bäumer<sup>2</sup>; C. Hoberg<sup>2</sup>; J. Savolainen<sup>1</sup>; G. Schwaab<sup>1</sup>; M. Havenith<sup>1</sup>; <sup>1</sup> Ruhr-Universität Bochum/D; <sup>2</sup> Ruhr Universität Bochum/D
- P 02.08 **THz spectroscopy of glycine: Spectral changes upon titration with HCl and NaOH**  
A. Bäumer<sup>1</sup>; D. Decka<sup>1</sup>; S. Schäfer<sup>1</sup>; H. Wirtz<sup>1</sup>; C. Hoberg<sup>1</sup>; J. Savolainen<sup>1</sup>; G. Schwaab<sup>1</sup>; M. Havenith<sup>1</sup>; <sup>1</sup> Ruhr-Universität Bochum/D
- P 02.09 **THz FTIR study of Ytterbium(III) Hydration**  
C. Klinkhammer<sup>1</sup>; G. Schwaab<sup>1</sup>; M. Havenith<sup>1</sup>; <sup>1</sup> Ruhr-Universität Bochum/D
- P 02.10 **Linking Viscosity and TD THz Spectra in Polyether Solvation**  
S. Schäfer<sup>1</sup>; H. Wirtz<sup>2</sup>; C. Hoberg<sup>2</sup>; J. Savolainen<sup>2</sup>; G. Schwaab<sup>2</sup>; M. Havenith<sup>2</sup>; <sup>1</sup> Ruhr-Universität Bochum/D; <sup>2</sup> Ruhr-Universität Bochum, Lehrstuhl für Physikalische Chemie II/D
- P 02.11 **THz spectroscopy of water confined in supramolecular clusters**  
F. Sebastiani<sup>1</sup>; N. Alzakhem<sup>2</sup>; L. Sofen<sup>2</sup>; G. Schwaab<sup>3</sup>; K. Raymond<sup>2</sup>; M. Havenith<sup>3</sup>; <sup>1</sup> Department of Physical Chemistry II, Ruhr Universität Bochum/D; <sup>2</sup> Department of Chemistry, University of California, Berkeley/USA; <sup>3</sup> Department of Physical Chemistry II, Ruhr Universität Bochum/D
- P 02.12 **NMR Deuteron Relaxation Time Experiments in Protic Ionic Liquids Beyond the Extreme Narrowing Limit**  
V. Overbeck<sup>1</sup>; V. Lehde<sup>2</sup>; A. Appelhagen<sup>3</sup>; D. Michalik<sup>3</sup>; R. Ludwig<sup>2</sup>; <sup>1</sup> University of Rostock/ Institute of Chemistry/D; <sup>2</sup> University of Rostock/ Institute of Chemistry/D; <sup>3</sup> Leibniz Institute for Catalysis at University Rostock/D
- P 02.13 **Principal components of the vibrational spectra of solvent mixtures**  
J. Kiefer<sup>1</sup>; M. Miciuk<sup>1</sup>; H. Schwietert<sup>1</sup>; F. Zehentbauer<sup>2</sup>; <sup>1</sup> Universität Bremen/D; <sup>2</sup> University of Strathclyde, Glasgow/UK
- P 02.14 **Ionicity of Ionic Liquids determined by PFG-STE NMR**  
D. Rauber<sup>1</sup>; F. Philippi<sup>1</sup>; R. Hempelmann<sup>1</sup>; <sup>1</sup> Saarland University, Saarbrücken/D
- P 02.15 **Analysis of perturbed H<sub>2</sub>O vibrations beyond Fourier transform**  
W. Langel<sup>1</sup>; N. Geist<sup>2</sup>; <sup>1</sup> Universität Greifswald/D; <sup>2</sup> Universität Greifswald/D

### Chemical Dynamics and Kinetics

- P 03.01 **Scattering of Formaldehyde from Au (111)**  
B. Krüger<sup>1</sup>; G. Park<sup>2</sup>; S. Meyer<sup>2</sup>; A. Wodtke<sup>2</sup>; T. Schäfer<sup>2</sup>; <sup>1</sup> Georg-August-Universität Göttingen/D; <sup>2</sup> Georg-August-Universität Göttingen, Institut für Physikalische Chemie/D
- P 03.02 **Following the Ultrafast Dynamics of a Bistable Intramolecular H-Transfer Switch by Time-Resolved Vibrational Spectroscopy**  
H. Böhnke<sup>1</sup>; J. Bahrenburg<sup>1</sup>; F. Temps<sup>1</sup>; <sup>1</sup> Christian-Albrechts-Universität zu Kiel/D
- P 03.03 **Nuclear motion is classical**  
I. Frank<sup>1</sup>; <sup>1</sup> Theoretische Chemie, Hannover/D
- P 03.04 **Ultrafast studies on luminescent mono- and dinuclear copper(I)-complexes**  
M. Grupe<sup>1</sup>; F. Bäppler<sup>1</sup>; F. Dietrich<sup>1</sup>; D. Volz<sup>2</sup>; S. Bräse<sup>3</sup>; M. Gerhards<sup>1</sup>; R. Diller<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Cynora GmbH, Bruchsal/D; <sup>3</sup> Karlsruhe Institute of Technology (KIT)/D
- P 03.05 **Photo-initiated dynamics of trans- and cis-ferulic acid in aqueous solutions**  
S. Wang<sup>1</sup>; S. Schatz<sup>1</sup>; H. Böhnke<sup>1</sup>; M. Stuhldreier<sup>1</sup>; T. Raeker<sup>1</sup>; B. Hartke<sup>1</sup>; J. Keppler<sup>1</sup>; K. Schwarz<sup>1</sup>; F. Renth<sup>1</sup>; F. Temps<sup>1</sup>; <sup>1</sup> Kiel University/D
- P 03.06 **Experimental and modeling investigation on fuel-structure-dependent reaction pathways in C<sub>2</sub>-flames**  
L. Ruwe<sup>1</sup>; L. Leon<sup>2</sup>; K. Moshammer<sup>3</sup>; L. Seidel<sup>2</sup>; N. Hansen<sup>4</sup>; F. Mauss<sup>2</sup>; K. Kohse-Höinghaus<sup>5</sup>; <sup>1</sup> Universität Bielefeld/D; <sup>2</sup> Brandenburg University of Technology, Cottbus/D; <sup>3</sup> Physikalisch Technische Bundesanstalt, Braunschweig/D; <sup>4</sup> Sandia National Laboratories, Livermore/USA; <sup>5</sup> Bielefeld University/D


**POSTER PROGRAMME**

- P 03.07 **The Photodissociation of the ortho- & para-Xylyl Radical, C<sub>8</sub>H<sub>9</sub>, Investigated by Velocity Map Imaging**  
K. Pachner<sup>1</sup>; I. Fischer<sup>1</sup>; <sup>1</sup> Universität Würzburg/D
- P 03.08 **Kinetic Investigations of the Pyrolysis and Oxidation of Dimethoxymethane**  
L. Golka<sup>1</sup>; C. Bänsch<sup>1</sup>; K. Wegner<sup>2</sup>; M. Olzmann<sup>1</sup>; <sup>1</sup> Karlsruher Institut für Technologie (KIT), Institut für Physikalische Chemie/D; <sup>2</sup> Karlsruhe Institute of Technology (KIT)/D
- P 03.09 **Ultrafast Vibrational and Electronic Dynamics of Coinage Metal-Phosphine Complexes in an Ion Trap and in Solution**  
S. Kruppa<sup>1</sup>; F. Bäppler<sup>1</sup>; Y. Nosenko<sup>1</sup>; S. Walg<sup>2</sup>; R. Diller<sup>1</sup>; W. Klopper<sup>3</sup>; C. Riehn<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Karl-Franzens-University Graz/A; <sup>3</sup> Karlsruhe Institute of Technology (KIT)/D
- P 03.10 **Intramolecular cooperativity in tetranuclear and 1D- polynuclear spin crossover complexes modeled with density functional theory**  
J. Wolny<sup>1</sup>; L. Scherthan<sup>2</sup>; V. Schünemann<sup>3</sup>; W. Klopper<sup>4</sup>; B. Schäfer<sup>5</sup>; M. Ruben<sup>5</sup>; <sup>1</sup> University of Kaiserslautern/D; <sup>2</sup> TU Kaiserslautern/D; <sup>3</sup> University of Kaiserslautern/D; <sup>4</sup> Karlsruhe Institute of Technology (KIT)/D; <sup>5</sup> KIT Karlsruhe/D
- P 03.11 **fs time-resolved UV/IR and UV/Vis Pump-Probe Studies on the Photochemistry of Benzocyclobutene-1,2-dione**  
M. Flock<sup>1</sup>; H. Schmitt<sup>1</sup>; I. Fischer<sup>1</sup>; X. Ma<sup>1</sup>; T. Brixner<sup>1</sup>; <sup>1</sup> Julius Maximilians University of Würzburg/D
- P 03.12 **Theoretical study of bond cleavage reactions in TEOS and TTIP**  
M. Marcinkowski<sup>1</sup>; H. Somnitz<sup>1</sup>; <sup>1</sup> Universität Duisburg-Essen/D
- P 03.13 **“Super”photoacid-Base-Complexes to Reveal Medium-Effects of Proton Transfer Reactions**  
A. Grandjean<sup>1</sup>; J. Menges<sup>1</sup>; D. Maus<sup>1</sup>; G. Jung<sup>1</sup>; <sup>1</sup> Saarland University, Saarbrücken/D
- P 03.14 **Search for Stronger Super-Photoacids**  
D. Maus<sup>1</sup>; A. Grandjean<sup>1</sup>; G. Jung<sup>1</sup>; <sup>1</sup> Saarland University, Saarbrücken/D
- P 03.15 **Influence of small ether addition on combustion-related intermediates and flame structure in premixed n-heptane flames**  
J. Wullenkord<sup>1</sup>; M. Zeng<sup>2</sup>; I. Graf<sup>1</sup>; K. Kohse-Höinghaus<sup>1</sup>; <sup>1</sup> Bielefeld University/D; <sup>2</sup> University of Science and Technology of China, Hefei/CN
- P 03.16 **Using FEL femtosecond pulses in the VUV to control dissociative/non-dissociative ionization of H<sub>2</sub>**  
F. Holzmeier<sup>1</sup>; M. Hervé<sup>1</sup>; M. Meyer<sup>2</sup>; T. Baumann<sup>2</sup>; A. Achner<sup>2</sup>; C. Callegari<sup>3</sup>; M. Di Fraia<sup>3</sup>; K. Prince<sup>3</sup>; R. Richter<sup>3</sup>; P. Finetti<sup>3</sup>; O. Plekan<sup>3</sup>; E. Roussel<sup>3</sup>; D. Gauthier<sup>3</sup>; F. Martín<sup>4</sup>; A. Palacios<sup>5</sup>; R. Bello<sup>5</sup>; H. Bachau<sup>6</sup>; D. Dowek<sup>1</sup>; <sup>1</sup> CNRS, Institut des Sciences Moléculaires d'Orsay (ISMO), University Paris-Sud, Orsay/F; <sup>2</sup> European XFEL, Hamburg/D; <sup>3</sup> Elettra-Sincrotrone Trieste/I; <sup>4</sup> Universidad Autónoma de Madrid/E; <sup>5</sup> Universidad Autonoma de Madrid/E; <sup>6</sup> Université de Bordeaux/F
- P 03.17 **Radiation Chemical Modification of Carbon Nanodots**  
A. Kahnt<sup>1</sup>; F. Plass<sup>1</sup>; <sup>1</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)/D
- P 03.18 **Effects of unsaturated methyl esters on soot precursors**  
M. Salamanca<sup>1</sup>; L. Ruwe<sup>1</sup>; K. Kohse-Höinghaus<sup>1</sup>; <sup>1</sup> Bielefeld University/D
- P 03.19 **Combustion Chemistry of Butane and Butene Isomers in an Atmospheric Pressure High-Temperature Laminar Flow Reactor – a Molecular-Beam Mass Spectrometric Study**  
D. Borodin<sup>1</sup>; <sup>1</sup> Georg-August-Universität Göttingen, Institute of Physical Chemistry/D
- P 03.20 **Lifetimes and energetics of the first electronically excited states of NaH<sub>2</sub>O from time-resolved photoelectron imaging**  
T. Gartmann<sup>1</sup>; B. Yoder<sup>1</sup>; E. Chasovskikh<sup>1</sup>; R. Signorelli<sup>1</sup>; <sup>1</sup> ETH Zürich/CH
- P 03.21 **Ps Time-Resolved Photoionisation of the S2 ( $\pi\pi^*$ ) State of Isolated Xanthone**  
H. Schmitt<sup>1</sup>; M. Flock<sup>1</sup>; I. Fischer<sup>1</sup>; <sup>1</sup> Julius Maximilians University of Würzburg/D
- P 03.22 **Optimization of the VIPER pulse sequence using coumarin 6**  
C. Neumann<sup>1</sup>; D. Kern-Michler<sup>2</sup>; L. van Wilderen<sup>2</sup>; J. von Cosel<sup>2</sup>; I. Burghardt<sup>2</sup>; J. Bredenbeck<sup>2</sup>; <sup>1</sup> Universität Frankfurt/D; <sup>2</sup> Goethe Universität Frankfurt am Main/D

- P 03.23 **Ultrafast Electronic Dynamics and Rotational Dephasing of Supramolecular Photocatalysts in an Ion Trap**  
C. Riehn<sup>1</sup>; D. Imanbaew<sup>1</sup>; J. Lang<sup>1</sup>; M. Gelin<sup>2</sup>; S. Kaufhold<sup>3</sup>; M. Pfeffer<sup>3</sup>; S. Rau<sup>3</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> TU München, Garching/D; <sup>3</sup> Universität Ulm/D
- P 03.24 **Improvement of continuous-wave ESR line broadening experiments of the electron self-exchange kinetics of activated processes in imidazolium based ionic liquids by means of binary mixtures**  
M. Berghold<sup>1</sup>; J. Bächle<sup>2</sup>; G. Grampp<sup>2</sup>; S. Landgraf<sup>2</sup>; <sup>1</sup> Graz University of Technology/A; <sup>2</sup> Institute of Physical and Theoretical Chemistry, Graz University of Technology/A
- P 03.25 **Reactivity of CO<sub>3</sub><sup>-</sup> with Atmospherically Relevant Acids**  
C. van der Linde<sup>1</sup>; W. Tang<sup>2</sup>; C. Siu<sup>2</sup>; M. Beyer<sup>1</sup>; <sup>1</sup> Universität Innsbruck/A; <sup>2</sup> City University Hong Kong/HK
- P 03.26 **Cold and controlled molecules for molecular imaging experiments**  
J. Küpper<sup>1</sup>; <sup>1</sup> Center for Free-Electron Laser Science, DESY and Universität Hamburg/D
- P 03.27 **Gas-phase reactivity of molybdenum clusters with dimethyl disulfide**  
A. Baloglu<sup>1</sup>; M. Beyer<sup>1</sup>; <sup>1</sup> University of Innsbruck/A

### Molecular Structure

- P 04.01 **The Microwave Spectrum of Methyl Methacrylate**  
S. Herbers<sup>1</sup>; D. Wachsmuth<sup>1</sup>; J. Grabow<sup>1</sup>; <sup>1</sup> Institut für physikalische Chemie und Elektrochemie, Gottfried Wilhelm Leibniz Universität, Hannover/D
- P 04.02 **Chemical control of the cis/trans equilibrium in N-monosubstituted amides – A possible intramolecular dispersion energy balance**  
B. Hartwig<sup>1</sup>; T. Forsting<sup>2</sup>; M. Suhm<sup>1</sup>; <sup>1</sup> Georg-August-Universität Göttingen, Institut für Physikalische Chemie/D; <sup>2</sup> Georg-August-Universität Göttingen/D
- P 04.03 **Furan microsolvation – from biofuels over double-blind challenges to polycyclic aromatic derivatives**  
A. Poblotzki<sup>1</sup>; H. Gottschalk<sup>1</sup>; R. Mata<sup>1</sup>; M. Suhm<sup>1</sup>; <sup>1</sup> Georg-August-Universität Göttingen, Institut für Physikalische Chemie/D
- P 04.04 **Pulling on the naphthol-anisole OH-O hydrogen bond with chemically tuned dispersion forces**  
A. Nejad<sup>1</sup>; A. Poblotzki<sup>1</sup>; M. Suhm<sup>1</sup>; <sup>1</sup> Georg-August-Universität Göttingen, Institut für Physikalische Chemie/D
- P 04.05 **Site-selective detection of iron vibrational modes in a trinuclear complex**  
I. Faus<sup>1</sup>; L. Scherthan<sup>1</sup>; S. Rackwitz<sup>1</sup>; J. Wolny<sup>1</sup>; A. Banerjee<sup>1</sup>; H. Kelm<sup>1</sup>; H. Krüger<sup>1</sup>; K. Schrage<sup>2</sup>; H. Wille<sup>2</sup>; V. Schünemann<sup>1</sup>; <sup>1</sup> University of Kaiserslautern/D; <sup>2</sup> Deutsches Elektronen Synchrotron DESY, Hamburg/D
- P 04.06 **Interaction of homo and heterometallic trinuclear complexes with light studied by Mössbauer spectroscopy**  
T. Bauer<sup>1</sup>; A. Omlor<sup>1</sup>; H. Auerbach<sup>1</sup>; K. Jenni<sup>1</sup>; M. Schmitz<sup>1</sup>; A. Banerjee<sup>1</sup>; H. Kelm<sup>1</sup>; H. Krüger<sup>1</sup>; B. Schäfer<sup>2</sup>; M. Ruben<sup>2</sup>; V. Schünemann<sup>1</sup>; <sup>1</sup> University of Kaiserslautern/D; <sup>2</sup> Karlsruhe Institute of Technology (KIT)/ Institute of Nanotechnology/D
- P 04.07 **Study of the self-reaction products of benzyl radicals via IR/UV ion-dip-spectroscopy**  
F. Hirsch<sup>1</sup>; P. Constantinidis<sup>1</sup>; I. Fischer<sup>1</sup>; A. Rijs<sup>2</sup>; <sup>1</sup> Universität Würzburg/D; <sup>2</sup> Radboud Universiteit, Nijmegen/NL
- P 04.08 **Exotic chemistry with ultracold Rydberg atoms**  
M. Peper<sup>1</sup>; H. Saßmannshausen<sup>2</sup>; F. Merkt<sup>2</sup>; J. Deiglmayr<sup>2</sup>; <sup>1</sup> ETH Zürich/CH; <sup>2</sup> ETH Zürich/CH
- P 04.09 **The role of dispersion interactions on the microsolvation of aromatic ethers**  
F. Dietrich<sup>1</sup>; D. Bernhard<sup>1</sup>; M. Fatima<sup>2</sup>; M. Luczak<sup>1</sup>; M. Burkhart<sup>1</sup>; M. Schnell<sup>2</sup>; M. Gerhards<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg/D
- P 04.10 **Photoelectron Spectroscopy of the three Picolyl Radical Isomers**  
E. Reusch<sup>1</sup>; F. Holzmeier<sup>2</sup>; P. Constantinidis<sup>1</sup>; P. Hemmerger<sup>3</sup>; I. Fischer<sup>1</sup>; <sup>1</sup> Julius-Maximilians Universität Würzburg/D; <sup>2</sup> Synchrotron SOLEIL, Gif Sur Yvette/F; <sup>3</sup> Paul Scherrer Institut (PSI), Villigen/CH


**POSTER PROGRAMME**

- P 04.11 **IR spectroscopy of cationic nickel ethanol clusters – variation of cluster size and solvation shell**  
M. Becherer<sup>1</sup>; D. Bellaire<sup>1</sup>; F. Dietrich<sup>1</sup>; M. Gerhards<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D
- P 04.12 **Reactivity Information from Experimental Electron Densities**  
M. Prosenc<sup>1</sup>; J. Klöckner<sup>2</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> Universität Hamburg/D
- P 04.13 **Spectroscopy and Kinetics of N<sub>2</sub> on Transition Metal Cluster Surfaces**  
S. Dillinger<sup>1</sup>; J. Mohrbach<sup>1</sup>; G. Niedner-Schatteburg<sup>1</sup>; <sup>1</sup> TU Kaiserslautern, Fachbereich Chemie/D
- P 04.14 **Validation of trimethylamine N-oxide (TMAO) force fields based on properties of aqueous TMAO solutions**  
J. Baz<sup>1</sup>; D. Markthaler<sup>1</sup>; J. Zemann<sup>2</sup>; J. Smiatek<sup>2</sup>; N. Hansen<sup>1</sup>; <sup>1</sup> Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart/D; <sup>2</sup> Institute for Computational Physics, University of Stuttgart/D
- P 04.15 **Systematic investigation of sign effects for methane and ethane in chirped femtosecond laser fields**  
V. Krein<sup>1</sup>; K. Weitzel<sup>1</sup>; <sup>1</sup> Philipps-Universität Marburg/D
- P 04.16 **Infrared spectroscopic investigations of N<sub>2</sub> adsorbed to cold Rhodium Iron alloy cluster cations**  
M. Klein<sup>1</sup>; A. Ehrhard<sup>1</sup>; J. Mohrbach<sup>1</sup>; S. Dillinger<sup>1</sup>; G. Niedner-Schatteburg<sup>1</sup>; <sup>1</sup> TU Kaiserslautern, Fachbereich Chemie/D
- P 04.17 **Precision measurements of the rovibrational energy-level structure of 4He<sub>2</sub><sup>+</sup>**  
L. Semeria<sup>1</sup>, P. Jansen<sup>1</sup>, J. Agner<sup>1</sup>, H. Schmutz<sup>1</sup>, F. Merkt<sup>1</sup>; <sup>1</sup> ETH Zürich/CH

### Experimental Techniques

- P 05.01 **Double-imaging fixed-photon-energy photoelectron/photoion coincidence (i<sup>2</sup>PEPICO) spectroscopy for combustion analysis**  
S. Schmitt<sup>1</sup>; J. Pieper<sup>1</sup>; J. Krüger<sup>2</sup>; G. Garcia<sup>2</sup>; L. Nahon<sup>2</sup>; W. Eisfeld<sup>1</sup>; A. Brockhinke<sup>1</sup>; K. Kohse-Höinghaus<sup>1</sup>; <sup>1</sup> Bielefeld University/D; <sup>2</sup> Synchrotron SOLEIL, Gif-sur-Yvette/F
- P 05.02 **Vibrational Blue Shift of coordinated N<sub>2</sub> in [Fe<sub>3</sub>O(OAc)<sub>6</sub>(N<sub>2</sub>)n]<sup>+</sup>: “Non Classical” Dinitrogen Complexes**  
J. Lang<sup>1</sup>; J. Mohrbach<sup>1</sup>; S. Dillinger<sup>1</sup>; J. Hewer<sup>1</sup>; G. Niedner-Schatteburg<sup>1</sup>; <sup>1</sup> TU Kaiserslautern, Fachbereich Chemie/D
- P 05.03 **Vapor-liquid Equilibria of Binary Mixtures of Imidazolium-Based Ionic Liquids with n-Alkyl Alcohols**  
M. Stuckenholz<sup>1</sup>; P. Carvalho<sup>2</sup>; J. Kiefer<sup>1</sup>; J. Coutinho<sup>2</sup>; W. Schröer<sup>1</sup>; B. Rathke<sup>1</sup>; <sup>1</sup> Universität Bremen/D; <sup>2</sup> University of Aveiro/P
- P 05.04 **Analytical Method Development for Monitoring the Extraction of Natural Components with Ionic Liquids**  
A. Dittmar<sup>1</sup>; M. Rocha<sup>1</sup>; D. Kerlé<sup>1</sup>; B. Rathke<sup>1</sup>; J. Kiefer<sup>1</sup>; <sup>1</sup> Universität Bremen/D
- P 05.05 **Piezo-electric detectors as a tool for determining the size of climate-relevant clusters in pulsed supersonic molecular beams**  
P. Saftien<sup>1</sup>; S. Fazli<sup>1</sup>; K. Lange<sup>2</sup>; W. Christen<sup>1</sup>; <sup>1</sup> Humboldt-Universität zu Berlin/D; <sup>2</sup> Sensor- und Lasertechnik, Neuenhagen/D
- P 05.06 **Nucleation Rates of Carbon-Dioxide Gashydrates**  
J. Castellanos Muñoz<sup>1</sup>; J. Kiefer<sup>1</sup>; B. Rathke<sup>1</sup>; <sup>1</sup> Technische Thermodynamik, Universität Bremen/D
- P 05.07 **Sub-Monolayer NIR-ew-CRD Spectroscopy: Picosecond Versus Continuous Wave Laser Excitation**  
A. Baumann<sup>1</sup>; I. Piller<sup>1</sup>; G. Friedrichs<sup>1</sup>; <sup>1</sup> Christian-Albrechts-Universität zu Kiel/D
- P 05.08 **Optical focusing of isolated particles for diffractive imaging experiments**  
S. Awel<sup>1</sup>; D. Horkel<sup>1</sup>; A. Rode<sup>2</sup>; X. Sun<sup>3</sup>; N. Roth<sup>4</sup>; R. Kirian<sup>5</sup>; J. Küpper<sup>6</sup>; H. Chapman<sup>6</sup>; <sup>1</sup> Center for Free-Electron Laser Science, DESY and The Hamburg Centre for Ultrafast Imaging/D; <sup>2</sup> Australian National University, Canberra/AUS; <sup>3</sup> Center for Free-Electron Laser Science, DESY, Hamburg/D; <sup>4</sup> Center for Free-Electron Laser Science, Hamburg/D; <sup>5</sup> Department of Physics, Arizona State University, Tempe/USA; <sup>6</sup> Center for Free-Electron Laser Science, DESY, The Hamburg Centre for Ultrafast Imaging and Universität Hamburg/D

- P 05.09 **Wavelength dependence observed in the ablation of Galvanoaluminium-Nickel Coatings on Steel by UV- and VIS-LIBS**  
M. Weimerskirch<sup>1</sup>; <sup>1</sup> Faculty of Physics, University of Vienna/A

- P 05.10 **Numerical simulations for characterizing and optimizing an aerodynamic lens**  
N. Roth<sup>1</sup>; S. Awel<sup>2</sup>; D. Horke<sup>2</sup>; J. Küpper<sup>3</sup>; <sup>1</sup> Center for Free-Electron Laser Science, DESY, Hamburg/D;  
<sup>2</sup> Center for Free-Electron Laser Science, DESY and The Hamburg Centre for Ultrafast Imaging/D; <sup>3</sup> Center for Free-Electron Laser Science, DESY, The Hamburg Centre for Ultrafast Imaging and Universität Hamburg/D

### Theoretical Techniques

- P 06.01 **How sodium determines the interactions between cationic protein sites and polyatomic anions**  
S. Kashef Ol Gheta<sup>1</sup>; A. Vila Verde<sup>1</sup>; <sup>1</sup> MPI für Kolloid- und Grenzflächenforschung, Potsdam/D
- P 06.02 **Conformational Dynamics of Glycoproteins**  
E. Schulze<sup>1</sup>; M. Stein<sup>1</sup>; <sup>1</sup> Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
- P 06.03 **2c-DFT calculations on [ReCl<sub>4</sub>(CN)<sub>2</sub>]<sub>2</sub><sup>-</sup> and [(PY<sub>5</sub>Me<sub>2</sub>)<sub>2</sub>Mn<sub>2</sub>ReCl<sub>4</sub>(CN)<sub>2</sub>]<sub>2</sub><sup>-</sup>: Effect of Spin Orbit Coupling beyond 2nd order**  
E. Kessler<sup>1</sup>; C. van Wüllen<sup>2</sup>; <sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> TU Kaiserslautern, Fachbereich Chemie/D
- P 06.04 **Broken symmetry approach for single-ion hyperfine tensors of oligonuclear transition metal complexes**  
C. Mehlich<sup>1</sup>; C. van Wüllen<sup>1</sup>; <sup>1</sup> TU Kaiserslautern, Fachbereich Chemie/D
- P 06.05 **Analysis of simulation protocols for the calculation of standard binding free energies**  
D. Markthaler<sup>1</sup>; J. Gebhardt<sup>1</sup>; N. Hansen<sup>2</sup>; <sup>1</sup> University of Stuttgart/D; <sup>2</sup> Universität Stuttgart/D
- P 06.06 **Nuclear dynamical correlation effects in X-ray spectroscopy from a time-domain perspective**  
S. Karsten<sup>1</sup>; S. Bokarev<sup>1</sup>; S. Ivanov<sup>1</sup>; O. Kühn<sup>1</sup>; <sup>1</sup> Rostock University/D
- P 06.07 **Open Boundary / Grand-Canonical Adaptive Resolution Simulations of Ionic Liquids**  
C. Krekeler<sup>1</sup>; L. Delle Site<sup>1</sup>; <sup>1</sup> Freie Universität Berlin/D
- P 06.08 **Fullerene in water: local microscopic structures v.s. quantum delocalization of atoms in space**  
A. Agarwal<sup>1</sup>; C. Clementi<sup>1</sup>; L. Delle Site<sup>1</sup>; <sup>1</sup> Freie Universität Berlin/D

### Solids and Nano-sized Matter

- P 07.01 **Electrical transport through monolayers of hybrid Pt-CdSe nanoparticles**  
C. Klinke<sup>1</sup>; <sup>1</sup> University of Hamburg/D
- P 07.02 **Organic nanofibers for optoelectronic devices**  
M. La Rosa<sup>1</sup>; C. Dosche<sup>1</sup>; J. Christoffers<sup>1</sup>; K. Al-Shamery<sup>1</sup>; <sup>1</sup> Carl von Ossietzky Universität Oldenburg/D
- P 07.03 **Synthesis and Spectroscopic Characterization of Ultrathin PbS Nanoplatelets**  
F. Manteiga Vázquez<sup>1</sup>; S. Kinge<sup>2</sup>; A. Houtepen<sup>1</sup>; J. Lauth<sup>1</sup>; L. Siebbeles<sup>1</sup>; <sup>1</sup> Delft University of Technology/NL;  
<sup>2</sup> Toyota Motor Europe, Zaventem/B
- P 07.04 **Photoelectrochemical Investigations of Hetero-Nanoparticle Based Gelstructures**  
J. Miethe<sup>1</sup>; F. Lübkemann<sup>2</sup>; J. Poppe<sup>2</sup>; N. Bigall<sup>2</sup>; <sup>1</sup> Leibniz Universität Hannover/D; <sup>2</sup> Leibniz Universität Hannover/  
Institut für Physikalische Chemie und Elektrochemie/D
- P 07.05 **Immobilization of Pyrene-based Photoacids**  
A. Clasen<sup>1</sup>; A. Kraegeloh<sup>2</sup>; G. Jung<sup>1</sup>; <sup>1</sup> Universität des Saarlandes, Saarbrücken/D; <sup>2</sup> INM – Leibniz Institute for  
New Materials, Saarbrücken/D
- P 07.06 **Platinum Nanoparticle Patterning of Graphene using Inkjet Printing**  
M. Goudarzi<sup>1</sup>; M. Osmic<sup>2</sup>; C. Dosche<sup>2</sup>; k. Al-Shamery<sup>2</sup>; <sup>1</sup> Uiniversity of Oldenburg/D; <sup>2</sup> Institute of Chemistry,  
Oldenburg/D


**POSTER PROGRAMME**

- P 07.07 **Growth of Noble Metal Domains on CdSe Nanoplatelets**  
A. Schlosser<sup>1</sup>; S. Naskar<sup>1</sup>; N. Bigall<sup>1</sup>; <sup>1</sup> Leibniz Universität Hannover/D
- P 07.08 **Structure and photophysical dynamics of the corona phase around fluorescent nanoparticles**  
E. Polo<sup>1</sup>; F. Mann<sup>1</sup>; S. Kruss<sup>2</sup>; <sup>1</sup> Georg-August-Universität Göttingen/D; <sup>2</sup> Universität Göttingen/D
- P 07.09 **Adaption of Cryogelation to Various Nanoparticle Systems**  
D. Müller<sup>1</sup>; A. Freytag<sup>1</sup>; N. Bigall<sup>1</sup>; <sup>1</sup> Leibniz Universität Hannover/D
- P 07.10 **Time-Resolved Step-Scan FTIR and Transient Absorption/Reflectivity Investigations on a Dinuclear Cu(I)-NHETPHOS-complex**  
M. Zimmer<sup>1</sup>; F. Dietrich<sup>1</sup>; F. Bäppeler<sup>1</sup>; M. Wallesch<sup>2</sup>; D. Volz<sup>3</sup>; S. Bräse<sup>2</sup>; R. Diller<sup>1</sup>; M. Gerhards<sup>1</sup>;  
<sup>1</sup> TU Kaiserslautern/D; <sup>2</sup> KIT Karlsruhe/D; <sup>3</sup> Cynora GmbH, Bruchsal/D
- P 07.11 **Preparation of amphiphilic Janus particles and their effect on emulsion properties**  
M. Rehosek<sup>1</sup>; F. Marlow<sup>1</sup>; <sup>1</sup> Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr/D
- P 07.12 **Thermoelectrics properties of bis-2-phenylethylamin-CuCl4, -MnCl4 and their mixed crystals**  
M. Schomber<sup>1</sup>; J. Park<sup>2</sup>; I. Oh<sup>3</sup>; G. Eckold<sup>1</sup>; <sup>1</sup> Georg-August-Universität Göttingen/D; <sup>2</sup> Heinz Mayer-Leibnitz Institut, München/D; <sup>3</sup> Korea Atomic Energy Research Institute, Daejeon/KOR
- P 07.13 **Investigation of iron and silicon oxide formation in single levitated micro droplets by Raman and X-Ray fluorescence spectroscopy**  
R. Dallinger<sup>1</sup>; J. Schenk<sup>1</sup>; E. Rühl<sup>1</sup>; <sup>1</sup> Freie Universität Berlin, Institut für Chemie und Biochemie, Physikalische und Theoretische Chemie/D
- P 07.14 **Surface-Enhanced Raman Spectroscopy on Single Gold Nanoantennas**  
S. Küpper<sup>1</sup>; M. König<sup>1</sup>; S. Schlücker<sup>1</sup>; <sup>1</sup> University Duisburg-Essen/D
- P 07.15 **Size effects in MgO cube hydration and dissolution**  
J. Schneider<sup>1</sup>; R. Schwaiger<sup>2</sup>; S. Baumann<sup>3</sup>; T. Berger<sup>1</sup>; G. Bourret<sup>1</sup>; O. Diwald<sup>1</sup>; <sup>1</sup> Chemistry and Physics of Materials, Paris-Lodron University Salzburg/A; <sup>2</sup> Institute for Applied Materials, Karlsruhe Institute of Technology/D; <sup>3</sup> Institute of Particle Technology, Friedrich-Alexander University Erlangen-Nürnberg/D
- P 07.16 **Converting PAHs into nano-GOs**  
J. Weippert<sup>1</sup>; V. Gewiese<sup>1</sup>; P. Huber<sup>1</sup>; A. Böttcher<sup>1</sup>; M. Kappes<sup>1</sup>; <sup>1</sup> KIT Karlsruhe/D
- P 07.17 **Localized Surface Plasmon Resonance of Anisotropic and Hollow Metal Chalcogenide Nanoparticles**  
R. Himstedt<sup>1</sup>; P. Rusch<sup>1</sup>; D. Hinrichs<sup>1</sup>; T. Kodanek<sup>1</sup>; T. Mohamed<sup>1</sup>; D. Dorfs<sup>1</sup>; <sup>1</sup> Leibniz Universität Hannover/D
- P 07.18 **Probing the morphology of non-IPR fullerene films by monitoring the sublimation of dimers**  
J. Weippert<sup>1</sup>; L. Hohmann<sup>1</sup>; A. Böttcher<sup>1</sup>; M. Kappes<sup>1</sup>; <sup>1</sup> KIT Karlsruhe/D
- P 07.19 **Tribochemically induced optical Property Changes in MgO-Nanoparticle Powders**  
T. Schwab<sup>1</sup>; D. Thomele<sup>1</sup>; O. Diwald<sup>1</sup>; <sup>1</sup> Paris-Lodron Universität Salzburg/A
- P 07.20 **Inkjet Printing of Aqueous Photoluminescent CdSe/CdS Nanorods on Conducting Surfaces**  
F. Lübkemann<sup>1</sup>; R. Anselmann<sup>2</sup>; T. Kodanek<sup>1</sup>; D. Dorfs<sup>1</sup>; N. Bigall<sup>1</sup>; <sup>1</sup> Leibniz Universität Hannover, Institute of Physical Chemistry and Electrochemistry/D; <sup>2</sup> Evonik Resource Efficiency GmbH, Marl/D
- P 07.21 **Explanation of the Optical Properties of Shape Anisotropic Noble Metal Nanoparticles**  
A. Knauer<sup>1</sup>; J. Köhler<sup>1</sup>; <sup>1</sup> TU Ilmenau/D

### Soft Matter and Polymers

- P 08.01 **High resolution micro-resonator for chemo-selective sensing in liquids**  
J. Menges<sup>1</sup>; P. Peiker<sup>2</sup>; S. Klingel<sup>2</sup>; H. Bart<sup>3</sup>; E. Oesterschulze<sup>2</sup>; <sup>1</sup> TU Kaiserslautern, Lehrstuhl für Thermische Verfahrenstechnik/D; <sup>2</sup> Physics and Technology of Nanostructures, University of Kaiserslautern/D; <sup>3</sup> Chair of Separation Science and Technology, University of Kaiserslautern/D

- P 08.02 **Immobilization of ionic liquids in PBI framework for HT-PEMFC applications**  
G. Skorikova<sup>1</sup>; R. Hempelmann<sup>1</sup>; <sup>1</sup> Universität des Saarlandes, Saarbrücken/D
- P 08.03 **Proton Transfer Events in Spatially Confined Media**  
E. Eisbein<sup>1</sup>; T. Lorenz<sup>1</sup>; G. Seifert<sup>1</sup>; J. Joswig<sup>1</sup>; <sup>1</sup> TU Dresden/D
- P 08.04 **Potassium ion conductivity through sulfonated poly(ether-ether)ketone**  
M. Schäfer<sup>1</sup>, P. Knauth<sup>2</sup>, K. Weitzel<sup>1</sup>; <sup>1</sup> Universität Marburg/D, <sup>2</sup> Aix-Marseille Université/F

### Surfaces and Interfaces

- P 09.01 **Dynamics of a solar cell hole transport material on mesoporous TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> thin films and in organic solvents**  
J. Hölzer<sup>1</sup>; M. Scholz<sup>1</sup>; K. Oum<sup>1</sup>; T. Lenzer<sup>1</sup>; <sup>1</sup> Universität Siegen, Physikalische Chemie/D
- P 09.02 **Surface Faceting and Reconstruction of Ceria Nanoparticles**  
C. Yang<sup>1</sup>; X. Yu<sup>1</sup>; S. Heißler<sup>1</sup>; A. Nefedov<sup>1</sup>; S. Colussi<sup>2</sup>; J. Llorca<sup>3</sup>; A. Trovarelli<sup>2</sup>; Y. Wang<sup>1</sup>; C. Wöll<sup>1</sup>; <sup>1</sup> Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology/D; <sup>2</sup> Dipartimento Politecnico, Università di Udine/I; <sup>3</sup> Institut de Techniques Energétiques and Centre for Research in Nanoengineering, Universitat Politècnica de Catalunya, Barcelona/E
- P 09.03 **CO-Adsorption on Pt/h-BN nanocluster arrays**  
F. Düll<sup>1</sup>; <sup>1</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)/D
- P 09.04 **Heat of adsorption of water on the Fe<sub>3</sub>O<sub>4</sub>(111) surface studied by density functional theory**  
X. Li<sup>1</sup>; J. Paier<sup>1</sup>; <sup>1</sup> Humboldt-Universität zu Berlin/D
- P 09.05 **Model catalytic studies of liquid organic hydrogen carriers: Triphenylamine / tricyclohexylamine on Pt(111)**  
J. Steinhauer<sup>1</sup>; P. Bachmann<sup>1</sup>; U. Bauer<sup>1</sup>; F. Späth<sup>1</sup>; F. Düll<sup>1</sup>; C. Papp<sup>1</sup>; H. Steinrück<sup>1</sup>; <sup>1</sup> FAU Erlangen-Nürnberg/D
- P 09.06 **pH- and reaction time influence on the sorption of Eu(III) on cement phases – a spectroscopy-based speciation analysis**  
K. Burek<sup>1</sup>; M. Kumke<sup>2</sup>; <sup>1</sup> Universität Potsdam/Physikalische Chemie/D; <sup>2</sup> Universität Potsdam/Physikalische Chemie/D
- P 09.07 **Untersuchung der Adhäsionskräfte des Meerwasserbakteriums Paracoccus seriniphilus an technisch relevanten Oberflächen**  
N. Davoudi<sup>1</sup>; L. Hofherr<sup>1</sup>; K. Huttenlochner<sup>1</sup>; C. Schlegel<sup>1</sup>; C. Müller-Renno<sup>1</sup>; R. Ulber<sup>1</sup>; C. Ziegler<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D
- P 09.08 **Kräfte zum lateralen Abscheren bakterieller Zellen von strukturierten Titanoberflächen**  
K. Huttenlochner<sup>1</sup>; N. Davoudi<sup>1</sup>; S. Christin<sup>2</sup>; L. Heimann<sup>1</sup>; M. Huster<sup>2</sup>; M. Bohley<sup>3</sup>; C. Müller-Renno<sup>1</sup>; J. Aurich<sup>3</sup>; R. Ulber<sup>2</sup>; C. Ziegler<sup>1</sup>; <sup>1</sup> TU Kaiserslautern, Abt. Biophysik/D; <sup>2</sup> TU Kaiserslautern, Institute of Bioprocess Engineering/D; <sup>3</sup> TU Kaiserslautern, Lehrstuhl für Fertigungstechnik und Betriebsorganisation/D
- P 09.09 **Hydroxyl Groups on Atomically Defined Cobalt Oxide Surfaces: An Infrared Reflection Absorption Spectroscopy Study of D<sub>2</sub>O and Deuterated Benzoic Acid on Co<sub>3</sub>O<sub>4</sub>(111), CoO(111), CoO(100) Films on Ir(100)**  
M. Schwarz<sup>1</sup>; T. Xu<sup>2</sup>; S. Mohr<sup>1</sup>; C. Hohner<sup>1</sup>; J. Libuda<sup>1</sup>; <sup>1</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)/D; <sup>2</sup> Universität Erlangen-Nürnberg (FAU)/D
- P 09.10 **Interaction of Ester-Functionalized Ionic Liquids with Atomically-Defined Oxide Surfaces: [POOMIM][NTf<sub>2</sub>] on Co<sub>3</sub>O<sub>4</sub>(111) and CoO(100)**  
T. Wähler<sup>1</sup>; T. Xu<sup>2</sup>; J. Schwegler<sup>3</sup>; P. Wasserscheid<sup>3</sup>; J. Libuda<sup>2</sup>; <sup>1</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Physikalische Chemie II, Langenzenn/D; <sup>2</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Physikalische Chemie II/D; <sup>3</sup> Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Chemische Reaktionstechnik (CRT)/D

## POSTER PROGRAMME

- P 09.11 **Dextran-Adsorption auf Oberflächen und Adsorption in Wechselwirkung mit Protein**  
C. Rösch<sup>1</sup>; K. Hüttenlochner<sup>1</sup>; J. Gertje<sup>1</sup>; S. Trautmann<sup>2</sup>; N. Umanskaya<sup>2</sup>; C. Müller-Renno<sup>1</sup>; M. Hannig<sup>2</sup>;  
<sup>1</sup> TU Kaiserslautern/Department of Physics/D; <sup>2</sup> University Hospital of the Saarland/Clinic of Operative Dentistry, Periodontology and Preventive Dentistry, Homburg/D
- P 09.12 **Patterning of tomato bushy stunt viruses (TBSV) on silicon investigated by scanning force and scanning electron microscopy**  
V. Rink<sup>1</sup>; M. Ani<sup>1</sup>; M. Braun<sup>2</sup>; K. Boonrood<sup>2</sup>; C. Müller-Renno<sup>1</sup>; G. Krczal<sup>2</sup>; C. Ziegler<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D;  
<sup>2</sup> RLP Agroscience GmbH, Neustadt/D
- P 09.13 **Fabrication and characterization of all-carbon nanocapacitors from graphene-carbon nanomembrane-graphene heterostructures**  
X. Zhang<sup>1</sup>; E. Marschewski<sup>1</sup>; T. Weimann<sup>2</sup>; P. Penner<sup>1</sup>; D. Emmrich<sup>1</sup>; P. Hinze<sup>2</sup>; A. Gölzhäuser<sup>1</sup>; <sup>1</sup> Universität Bielefeld/D; <sup>2</sup> Physikalisch-Technische Bundesanstalt (PTB), Braunschweig/D
- P 09.14 **Synthesis, Metalation and Structures of Tetrapyrroles at Interfaces**  
M. Zugermeier<sup>1</sup>; M. Chen<sup>1</sup>; H. Drescher<sup>1</sup>; L. Heuplick<sup>1</sup>; B. Klein<sup>1</sup>; C. Krug<sup>1</sup>; M. Liebold<sup>1</sup>; F. Niefeld<sup>1</sup>; L. Ruppenthal<sup>1</sup>;  
M. Schmid<sup>1</sup>; P. Schweyen<sup>2</sup>; H. Zhou<sup>1</sup>; M. Bröring<sup>2</sup>; J. Sundermeyer<sup>1</sup>; J. Gottfried<sup>1</sup>; <sup>1</sup> Philipps-Universität Marburg/D;  
<sup>2</sup> TU Braunschweig/D
- P 09.15 **Temperature dependent interaction of colloidal metal nanoparticles with oxide supports**  
M. Siemer<sup>1</sup>; L. Mohrhusen<sup>1</sup>; M. Osmić<sup>1</sup>; J. Kolny-Olesiak<sup>1</sup>; K. Al-Shamery<sup>1</sup>; <sup>1</sup> Carl von Ossietzky Universität Oldenburg/D
- P 09.16 **Adsorption of single molecules and dimers of acetic acid on hexagonal and cubic ice I surfaces: A quantum chemical study**  
H. Somnitz<sup>1</sup>; <sup>1</sup> University of Duisburg-Essen, Essen/D
- P 09.17 **Investigating the Water-Titanium Dioxide Interface using Sum Frequency Generation Spectroscopy**  
S. Schlegel<sup>1</sup>; S. Hosseinpour<sup>1</sup>; M. Gebhard<sup>2</sup>; A. Devi<sup>3</sup>; E. Backus<sup>1</sup>; <sup>1</sup> Max-Planck-Institut für Polymerforschung, Mainz/D; <sup>2</sup> Ruhr-Universität Bochum/D; <sup>3</sup> Ruhr-Universität Bochum/D
- P 09.18 **Functional Carbon Nanomembranes for CryoTEM Imaging of Biological Samples**  
Z. Tang<sup>1</sup>; J. Scherr<sup>2</sup>; A. Winter<sup>1</sup>; C. Neumann<sup>1</sup>; D. Rhinow<sup>3</sup>; A. Terfort<sup>2</sup>; A. Turchanin<sup>1</sup>; <sup>1</sup> Friedrich Schiller University Jena/D; <sup>2</sup> Goethe University Frankfurt/D; <sup>3</sup> Max Planck Institute of Biophysics, Frankfurt/D
- P 09.19 **A Neural Network Potential for the Simulation of Copper Clusters on Zinc Oxide**  
M. Paleico<sup>1</sup>; J. Behler<sup>1</sup>; <sup>1</sup> Lehrstuhl für Theoretische Chemie, Ruhr University Bochum/D
- P 09.20 **Ullmann Coupling on Coinage Metal Surfaces**  
C. Krug<sup>1</sup>; M. Chen<sup>1</sup>; Q. Fan<sup>1</sup>; J. Kuttnér<sup>1</sup>; M. Schmid<sup>1</sup>; G. Hilt<sup>1</sup>; J. Zhu<sup>2</sup>; J. Gottfried<sup>1</sup>; <sup>1</sup> Philipps-Universität Marburg/D; <sup>2</sup> University of Science and Technology of China, Hefei/CN
- P 09.21 **Eu(III) as an Optical Probe for Sorption Processes on Bentonite**  
S. Mc Gee<sup>1</sup>; S. Eidner<sup>1</sup>; M. Kumke<sup>1</sup>; <sup>1</sup> Universität Potsdam/Physikalische Chemie/D
- P 09.22 **LEED-FTIR-DFT investigation of a two-dimensional mixed phase  $\text{CO}_2 \cdot \text{C}_2\text{H}_2$  on the KCl(100) surface**  
J. Vogt<sup>1</sup>; <sup>1</sup> University of Magdeburg/D
- P 09.23 **What do ligands do to supported silver clusters**  
A. Kartouzian<sup>1</sup>; T. Lünkens<sup>2</sup>; A. Von Weber<sup>2</sup>; M. Jakob<sup>2</sup>; T. Lelaidier<sup>2</sup>; U. Heiz<sup>2</sup>; <sup>1</sup> TU München, Garching/D;  
<sup>2</sup> TU München, Lehrstuhl für Physikalische Chemie, Garching/D
- P 09.24 **Corrosion of Concrete by Water-Induced Metal-Proton Exchange**  
N. Giraudo<sup>1</sup>; P. Thissen<sup>2</sup>; <sup>1</sup> Karlsruhe Institut für Technologie (KIT)/D; <sup>2</sup> Karlsruhe Institute of Technology (KIT)/D
- P 09.25 **HREELS Study of Adsorbate-Induced Charge Accumulations and Collective Excitations at Metal/Organic Interfaces:  $\text{F}_4\text{TCNQ}/\text{Au}(111)$  and  $\text{TCNQ}/\text{Au}(111)$**   
F. Maaß<sup>1</sup>; D. Gebert<sup>1</sup>; P. Tegeder<sup>1</sup>; <sup>1</sup> Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg/D

**P 09.26 Template-Controlled On-Surface Synthesis of Macrocycles**

Q. Fan<sup>1</sup>; C. Wang<sup>2</sup>; T. Wang<sup>2</sup>; J. Zhu<sup>2</sup>; M. Chen<sup>1</sup>; M. Zugermeier<sup>1</sup>; C. Krug<sup>1</sup>; J. Kuttner<sup>1</sup>; G. Hilt<sup>1</sup>; W. Hieringer<sup>3</sup>; J. Gottfried<sup>1</sup>; <sup>1</sup> Fachbereich Chemie, Philipps-Universität Marburg/D; <sup>2</sup> National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei/CN; <sup>3</sup> Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg/D

**P 09.27 2H-Tetraphenylprophyrin adsorption on TiO<sub>2</sub> nanoparticles**

J. Schneider<sup>1</sup>; T. Berger<sup>1</sup>; O. Diwald<sup>1</sup>; <sup>1</sup> Chemistry and Physics of Materials, Paris-Lodron University Salzburg/A

**P 09.28 Proton Exchange Reactions on Wollastonite as model surface of Calcium-Silicates – Investigations with UHV-IRRAS**

C. Natzeck<sup>1</sup>; P. Weidler<sup>1</sup>; C. Woell<sup>1</sup>; P. Thissen<sup>1</sup>; <sup>1</sup> Karlsruher Institut für Technologie (KIT) - IFG/D

**P 09.29 Water adsorption on Fe<sub>2</sub>O<sub>3</sub>(0001) probed by IR-spectroscopy**

L. Schöttner<sup>1</sup>; A. Nefedov<sup>1</sup>; Y. Wang<sup>1</sup>; C. Wöll<sup>1</sup>; <sup>1</sup> Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology/D

**P 09.30 Preparation of manganese and manganese oxide clusters on graphene/Ir(111)**

S. Mauthe<sup>1</sup>; T. Bernhardt<sup>1</sup>; <sup>1</sup> University of Ulm/D

**P 09.31 Photooxidation of small ketone molecules on Titanium dioxide**

E. Artmann<sup>1</sup>; F. Knall<sup>1</sup>; T. Bernhardt<sup>1</sup>; <sup>1</sup> University of Ulm/D

**P 09.32 Growth and decay of Co islands on NiAl(110): A fast –STM and XPS Study**

A. Pathan<sup>1</sup>; <sup>1</sup> Ruhr Universität Bochum/D

**P 09.33 Changing interfaces: photoluminescence ZnO nanoparticle powders in different aqueous environments**

K. Kocsis<sup>1</sup>; M. Niedermaier<sup>1</sup>; V. Kasparek<sup>2</sup>; J. Bernardi<sup>3</sup>; T. Berger<sup>1</sup>; O. Diwald<sup>1</sup>; <sup>1</sup> University of Salzburg/A; <sup>2</sup> Brno University of Technology/CZ; <sup>3</sup> Vienna University of Technology/A

**P 09.34 Supraparticles based on Silica and Prepared by Evaporation - Shape Control and their Use as Self-Propelling Particles**

M. Sperling<sup>1</sup>; V. Spiering<sup>1</sup>; E. Oguztürk<sup>1</sup>; H. Kim<sup>2</sup>; O. Velev<sup>3</sup>; M. Gradzielski<sup>1</sup>; <sup>1</sup> TU Berlin/D; <sup>2</sup> North Carolina State University, Raleigh/USA; <sup>3</sup> North Carolina State University, Raleigh/D

**P 09.35 Entwicklung und Charakterisierung selbst-schwimmender Mikrokapseln mit biologischem Vorbild**

A. Froin<sup>1</sup>; H. Rehage<sup>1</sup>; <sup>1</sup> TU Dortmund/D

**Biophysical Chemistry****P 10 Posters of the topic „Biophysical Chemistry“ are shifted to the „Main Topic – Physical Chemistry for Life Sciences“****Catalysis****P 11.01 Model Catalytic Study of the Dehydrogenation of Indole Derivatives on Atomically Clean Pt(111) Single Crystals by Infrared Reflection-Absorption Spectroscopy**

M. Bertram<sup>1</sup>; M. Schwarz<sup>1</sup>; T. Nascimento Silva<sup>1</sup>; T. Döpper<sup>1</sup>; A. Görling<sup>1</sup>; J. Libuda<sup>1</sup>; <sup>1</sup> University of Erlangen-Nürnberg, Erlangen/D

**P 11.02 Adsorption of acetone on TiO<sub>2</sub> rutile(110)**

J. Kräuter<sup>1</sup>; M. Osmić<sup>1</sup>; K. Al-Shamery<sup>1</sup>; <sup>1</sup> Carl von Ossietzky University Oldenburg/D

**P 11.03 Single-Molecule Analysis of Fluorescent Catalysts**

C. Hoffmann<sup>1</sup>; M. Metzinger<sup>1</sup>; G. Jung<sup>1</sup>; <sup>1</sup> Saarland University, Saarbrücken/D

**P 11.04 Characterization of active iron sites in Fe-ZSM-5 catalysts using Mössbauer spectroscopy**

P. Kydala Ganeshan<sup>1</sup>; H. Huang<sup>1</sup>; I. Ellmers<sup>2</sup>; R. Pérez Vélez<sup>3</sup>; A. Brückner<sup>3</sup>; W. Grünert<sup>2</sup>; V. Schünemann<sup>1</sup>;

<sup>1</sup> Department of Physics, University of Kaiserslautern/D; <sup>2</sup> Lehrstuhl Technische Chemie, Ruhr-Universität Bochum/D; <sup>3</sup> Leibniz-Institut für Katalyse e. V., Rostock/D


**POSTER PROGRAMME**

- P 11.05 **Infrared spectroelectrochemical and infrared spectroscopic investigations of the iron catalyzed carbon dioxide reduction**  
E. Oberem<sup>1</sup>; A. Rosas-Hernández<sup>2</sup>; S. Fischer<sup>1</sup>; R. Francke<sup>1</sup>; M. Römelt<sup>3</sup>; R. Ludwig<sup>1</sup>; <sup>1</sup> Universität Rostock, Institut für Chemie/D; <sup>2</sup> Leibniz-Institut für Katalyse, Rostock/D; <sup>3</sup> Ruhr-Universität Bochum/D
- P 11.06 **Metal Nanoparticle-Catalyzed Reduction Using Borohydride in Aqueous Media: A Kinetic Analysis of the Surface Reaction by Microfluidic SERS**  
R. Grzeschik<sup>1</sup>; W. Xie<sup>1</sup>; S. Schlücker<sup>1</sup>; <sup>1</sup> University Duisburg-Essen/D
- P 11.07 **Activation of small organic molecules by size selected transition metal clusters (n = 2-8) in the gas phase**  
J. Meyer<sup>1</sup>; M. Lembach<sup>1</sup>; P. Boden<sup>1</sup>; G. Niedner-Schatteburg<sup>1</sup>; <sup>1</sup> TU Kaiserslautern/D
- P 11.08 **Methanol Synthesis from Industrial CO<sub>2</sub> Sources**  
H. Ruland<sup>1</sup>; M. Bukhtiyarova<sup>1</sup>; K. Kähler<sup>1</sup>; R. Schlögl<sup>1</sup>; <sup>1</sup> Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D
- P 11.09 **On the role of interfacial hydrogen bonds in “On-Water” catalysis**  
K. Karhan<sup>1</sup>; R. Khaliullin<sup>2</sup>; T. Kühne<sup>1</sup>; <sup>1</sup> Universität Paderborn (TMC)/D; <sup>2</sup> McGill University, Montreal/CDN
- P 11.10 **Mechanism of the Intrinsic Arginine Finger in Heterotrimeric G-Proteins Investigated via Experimental and Theoretical FTIR Spectroscopy**  
D. Mann<sup>1</sup>; K. Gerwert<sup>2</sup>; C. Kötting<sup>3</sup>; <sup>1</sup> Ruhr University Bochum/D; <sup>2</sup> Ruhr University Bochum, Department of Biophysics/D; <sup>3</sup> Ruhr-University Bochum, Department of Biophysics/D
- P 11.11 **Oxygen species relevant for ethylene epoxidation on silver: new XPS assignment to unreconstructed atomic O**  
E. Carboni<sup>1</sup>; T. Jones<sup>2</sup>; T. Rocha<sup>3</sup>; S. Piccinin<sup>4</sup>; A. Knop-Gericke<sup>2</sup>; R. Schlögl<sup>2</sup>; <sup>1</sup> Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Inorganic Chemistry c/o Helmholtz Zentrum Berlin für Materialien und Energie, Berlin/D; <sup>2</sup> Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Inorganic Chemistry, Berlin/D; <sup>3</sup> Laboratório Nacional de Luz Síncrotron - LNLS/CNPEM, Campinas/BR; <sup>4</sup> CNR-IOM DEMOCRITOS, Consiglio Nazionale delle Ricerche-Istituto Officina dei Materiali, c/o SISSA, Trieste/I
- P 11.12 **Water oxidation reaction with manganese oxide clusters**  
N. Zimmermann<sup>1</sup>; S. Lang<sup>1</sup>; T. Bernhardt<sup>1</sup>; <sup>1</sup> University of Ulm/D
- P 11.13 **A Comprehensive Study of Novel Copper(I) Photosensitizers Containing P<sup>N</sup>-Ligands**  
R. Giereth<sup>1</sup>; M. Karnahl<sup>1</sup>; S. Tschierelei<sup>2</sup>; <sup>1</sup> Universität Stuttgart/D; <sup>2</sup> Universität Ulm/D

### Electrochemistry and Energy

- P 12.01 **Energy Storage in Strained Organic Molecules: In-Situ IR Spectroscopy During Photoelectrochemical Conversion Between Norbornadiene and Quadricyclane**  
F. Waidhas<sup>1</sup>; F. Faisal<sup>2</sup>; O. Brummel<sup>2</sup>; M. Schwarz<sup>2</sup>; T. Nascimento Silva<sup>2</sup>; J. Libuda<sup>2</sup>; <sup>1</sup> FAU Erlangen-Nürnberg/D; <sup>2</sup> FAU Erlangen-Nürnberg/D
- P 12.02 **Single Particle Interactions on Microelectrode Surfaces**  
A. Alshalfouh<sup>1</sup>; G. Wittstock<sup>2</sup>; C. Dosche<sup>2</sup>; <sup>1</sup> Carl von Ossietzky University Oldenburg/D; <sup>2</sup> Carl von Ossietzky Universität Oldenburg/D
- P 12.03 **Characterization and improvement of the active materials in the vanadium redox flow battery**  
K. Weißhaar<sup>1</sup>; H. Natter<sup>1</sup>; R. Hempelmann<sup>1</sup>; <sup>1</sup> Saarland University, Saarbrücken/D
- P 12.04 **Modeling and multicriteria optimization of new electrosynthesis processes**  
M. von Kurnatowski<sup>1</sup>; P. Klein<sup>1</sup>; M. Bortz<sup>1</sup>; <sup>1</sup> Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern/D
- P 12.05 **Enhanced Photo-response of FeS<sub>2</sub> Films: The Role of Marcasite-Pyrite Phase Junctions**  
L. Wu<sup>1</sup>; N. Dzade<sup>2</sup>; L. Gao<sup>1</sup>; E. Hensen<sup>1</sup>; N. De Leeuw<sup>2</sup>; J. Hofmann<sup>1</sup>; <sup>1</sup> TU Eindhoven/NL; <sup>2</sup> Utrecht University/NL
- P 12.06 **Investigations on an improved state-of-charge indicator for the all-vanadium redox flow battery**  
J. Geiser<sup>1</sup>; H. Natter<sup>1</sup>; R. Hempelmann<sup>1</sup>; <sup>1</sup> Universität des Saarlandes, Saarbrücken/D

- P 12.07 **Electro-catalytic CO Oxidation on UHV-Prepared Pt/Co<sub>3</sub>O<sub>4</sub>(111) Model Catalysts Studied by Electrochemical Infrared Reflection Absorption Spectroscopy**  
C. Stumm<sup>1</sup>; M. Bertram<sup>1</sup>; F. Faisal<sup>1</sup>; O. Brummel<sup>1</sup>; J. Libuda<sup>1</sup>; <sup>1</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)/D
- P 12.08 **Long-term stability of the oxygen exchange kinetics of La<sub>0.6</sub>Sr<sub>0.4</sub>CoO<sub>3</sub> and La<sub>2</sub>NiO<sub>4</sub> against Cr- and Si-poisoning**  
W. Sittl<sup>1</sup>; E. Bucher<sup>1</sup>; A. Egger<sup>1</sup>; N. Schrödl<sup>1</sup>; <sup>1</sup> Montanuniversität Leoben/A
- P 12.09 **Synthesis of LiMnPO<sub>4</sub> with titanate doping**  
L. Esmezjan<sup>1</sup>; S. Indris<sup>2</sup>; H. Ehrenberg<sup>2</sup>; <sup>1</sup> Karlsruhe Institute of Technology (KIT)/D; <sup>2</sup> Karlsruhe Institute of Technology (KIT)/D
- P 12.10 **Introducing photoactive metal-complexes in carbon nanomembranes**  
M. Küllmer<sup>1</sup>; P. Endres<sup>1</sup>; A. Winter<sup>2</sup>; F. Herrmann-Westendorf<sup>1</sup>; M. Presselt<sup>1</sup>; A. Winter<sup>1</sup>; U. Schubert<sup>1</sup>; B. Dietzek<sup>1</sup>; A. Turchanin<sup>1</sup>; <sup>1</sup> Friedrich-Schiller-Universität/D; <sup>2</sup> Friedrich-Schiller-Universität Jena/D
- P 12.11 **Ionic and electronic conductivity of bulk and thin film Li<sub>2</sub>O**  
S. Lörger<sup>1</sup>; R. Usiskin<sup>1</sup>; J. Maier<sup>1</sup>; <sup>1</sup> Max Planck Institute for Solid State Research, Stuttgart/D
- P 12.12 **Defect interactions in the CeO<sub>2</sub>-ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub> solid solution**  
S. Grieshammer<sup>1</sup>; <sup>1</sup> Forschungszentrum Jülich GmbH, Aachen/D
- P 12.13 **Anion intercalation electrode for high-voltage semi-solid flow batteries**  
Z. Huang<sup>1</sup>; R. Hempelmann<sup>1</sup>; R. Chen<sup>1</sup>; <sup>1</sup> Transfercentre Sustainable Electrochemistry, Saarland University, Saarbrücken/D
- P 12.14 **Ionic liquid based aqueous electrolytes for redox flow battery**  
Y. Zhang<sup>1</sup>; R. Hempelmann<sup>1</sup>; R. Chen<sup>1</sup>; <sup>1</sup> Transfercentre Sustainable Electrochemistry, Saarland University, Saarbrücken/D

### Industrial Applications

- P 13.01 **Component Integrity Assessment by CT and PTR-QiTof**  
M. Mlynek<sup>1</sup>; F. Rehme<sup>1</sup>; V. Hüllen<sup>1</sup>; <sup>1</sup> Roche Diabetes Care GmbH, Mannheim/D
- P 13.02 **Investigation of the layer thickness- and wavelength-dependence of laser stratigraphy on Cu and Ni coatings using LIBS**  
E. Paulis<sup>1</sup>; U. Pacher<sup>2</sup>; M. Weimerskirch<sup>2</sup>; T. Nagy<sup>2</sup>; W. Kautek<sup>2</sup>; <sup>1</sup> University of Vienna/A; <sup>2</sup> University of Vienna/A

SOCIAL PROGRAMME

## Thursday, 25 May 2017

19:30 – 22:30 **Welcome Reception****Price: 10 € (incl. 19% VAT) nominal charge**

## Friday, 26 May 2017

10:30 **Guided tour in the Japanese Garden**

Guided Tour in the Japanese Garden including a visit of the historic tea and guest-house.

**Registration necessary, max. 25 participants, fee 16 €**

With about 13.500 sqm the Japanese Garden Kaiserslautern has become the largest Japanese Garden in Europe and the first of this kind in Rhineland-Palatinate. Not only its size is noteworthy but also its genesis and unique atmosphere are impressive. Just ten years after the foundation of the „Japanese Garden Association Kaiserslautern“ in 1997, an exotic garden paradise accessible to the public was designed right in the heart of Kaiserslautern’s city center and in close cooperation between municipal authorities and committed citizens. The garden project can therefore be marked as one of the first public-private-partnership cooperations in the field of landscape architecture in Germany.

12:00 **Lunch at the historic Spinnrädl**

Optional lunch will take place at the historic restaurant „Spinnrädl“ (at your own expenses) Kaiserslautern’s historic Spinnrädl restaurant was first mentioned on a map dating back to 1742. It is one of the oldest surviving timber-framed houses in the city and is located in the city center.

12:05 – 13:05 **Women’s Networking Lunch**

(Building 46, Room 267)

Keynote Speaker:

**Prof. Dr. Swetlana Schauermann**, CAU Kiel.**Price: 12 € (incl. 19% VAT) nominal charge**

The number of participants is limited to 50.

The Bunsen Society invites all women to this fourth Women’s Networking Lunch at the Bunsentagung 2017.

Join us for a lunch and get to know other successful women in our scientific community. This is a unique networking opportunity. The Women’s Networking Lunch enables female scientists, talented and eager students as well as company representatives to interact in a relaxed environment. This Lunch allows attendees to expand their professional network, to collaborate with peers, to share their personal and business experiences and to exchange opinions in an informal setting.

We truly look forward to welcoming you at the Women’s Networking Lunch and to ask you to register for it jointly with your conference registration.

The organisers, Yvonne Joseph & Melanie Schnell

14:00 **Count Palatinate Hall & underground passages****Registration necessary, max. 25 participants, fee 10 €**

The tour starts with a visit of the Count Palatinate Hall in the former Casimir Castle including the underground passages. Afterwards, your city guide will lead you to the “Schillerplatz” as well as to the Collegiate Church, considered to be the most significant late Gothic hall church in southwestern Germany. Next, you’ll walk through the old part of town and visit the Stadtmuseum (city museum). The city walk ends at the Emperor’s Fountain, which shows representations of historical and present-day Kaiserslautern in a light-hearted way.

18:15 – 21:15 **Poster Session & Poster Dinner**

Mensa (Building 30)

The Poster Session allows for in-depth exchange of latest research achievements and developments in an informal atmosphere while enjoying food and drinks with friends and colleagues.

**Admission is free, but advance online registration is requested.**

Please tick the appropriate box on the online registration form.

**REGISTRATION FEES<sup>1)</sup>****Registration fees until 3 March 2017**

Personal Members of the German Bunsen Society	260 €
Non-Members	335 €
Students <sup>2)</sup>	50 €
Students Non-member <sup>2)</sup>	100 €
Accompanying Person <sup>3)</sup>	65 €

**Late registrations after 3 March 2017 are subject to an additional fee of 25 € (except for accompanying person).**

1) No VAT requested according to § 4.22 USTG

2) Proof of status required (valid student ID or confirmation by the supervising professor).

3) Only participation to the Opening Ceremony, Opening Lecture and Welcome Dinner on 25 May 2017 and the Poster Session and Poster Dinner on 26 May 2017 are included, no entrance to the scientific lecture (incl. 19% VAT).

The conference ticket includes an electronic book of abstracts to be downloaded in advance (a printed version can be ordered with your registration for an additional fee of 10 €), the list of participants, meals and beverages during the poster session (online registration in advance is requested) and the coffee breaks.

**Lunches are not included in the registration fee.**

**REGISTRATION**

Please register online at [www.bunsentagung.de](http://www.bunsentagung.de).

Registration is open, subject to capacity of the lecture rooms, up to the beginning of the conference. Publication deadline of the list of participants is **3 May 2017**. It is not guaranteed that registrations received later will appear in the list.

**PAYMENT**

Due to organisational constraints we can only accept payment by credit or debit card (debit card only for german accounts). You will receive an invoice by general mail after your registration has been booked.

**CANCELLATION**

**Only written cancellations will be accepted** (letter, fax or e-mail) and are subject to 30 € administrative fee for cancellation made before **3 May 2017**. Later cancellations will be subject to a charge equal to 80% of the registration fee. From the conference date on, no refund is possible. If the event is cancelled by the German Bunsen Society, the full fees will be refunded. Any further claims for compensation are excluded.

**ACCOMMODATION**

You can access a list of hotels offering room allotments to the conference attendees on the conference website [www.bunsentagung.de](http://www.bunsentagung.de), via the item "Accommodation".

Participants should make their reservations with the hotel directly. Please provide the keyword "Bunsentagung 2017" for a special rate. We highly recommend to book your accommodation as early as possible.



## GENERAL INFORMATION

### VENUE

[\(Map on page 90\)](#)

Technische Universität Kaiserslautern  
Building 42, 46 and 30  
67663 Kaiserslautern

### HOW TO REACH THE VENUE

On the conference website [www.bunsentagung.de](http://www.bunsentagung.de), under the menu "Venue", you'll find a link to the route description to the Technische Universität Kaiserslautern.

#### Parking Information:

Parking space near the conference venue is limited. We highly recommend visitors to reach the venue by public transport.

### OPENING HOURS ON-SITE CONFERENCE OFFICE

[\(Building 42\)](#)

Thursday, 25 May 2017	11:00 – 19:30
Friday, 26 May 2017	08:00 – 18:00
Saturday, 27 May 2017	08:00 – 16:00

### CONTACTS

For information on conference, lecture and poster programme, registration and book of abstracts, please contact:

Mr. Matthias Neumann  
DECHEMA e.V.  
Theodor-Heuss-Allee 25  
60486 Frankfurt am Main/D

Phone: +49 (0)69 7564-254  
Fax: +49 (0)69 7564-176  
E-mail: [bunsentagung@dechema.de](mailto:bunsentagung@dechema.de)

For information on meetings of the German Bunsen Society, student grants, awards and exhibitors/sponsoring:

Deutsche Bunsen-Gesellschaft für physikalische Chemie e.V.  
German Bunsen Society for physical Chemistry  
Varrentrappstr. 40-42  
60486 Frankfurt am Main/D

Phone: +49 (0)69 7917-362  
Fax: +49 (0)69 7917-1362  
E-mail: [geschaefsstelle@bunsen.de](mailto:geschaefsstelle@bunsen.de)  
Internet: [www.bunsen.de](http://www.bunsen.de)

### CONFERENCE LANGUAGES

The official languages of the conference are English and German. The opening, award and funding sessions will be in German only (The opening lecture will be given in English). Authors are expected to give their presentation (oral or poster) in the language used in the title published in the conference programme.

**PLEASE NOTE:** Simultaneous translation will not be available.

### CHILD CARE

The Bunsentagung offers the opportunity for child care service to parents of small children during the event. Interested parents are requested to complete the specific part with their online registration.

### INTERNET SERVICE

Free internet access will be provided via the eduroam service (<https://www.eduroam.org>) or the TU Kaiserslautern network for all participants during the conference.

**POSTER SESSION, POSTER DINNER AND POSTER AWARDS****Friday, 26 May 2017****18:15 – 21:15**

There will be a dedicated “Poster Session” on Friday, 26 May 2017 from 18:15 – 21:15. The session will be split between even poster numbers (from 18:15 – 19:45) and odd poster numbers (from 19:45 – 21:15). Each presenting author will have 1,5 hours to present his/her poster. **Authors are expected to be present at their own poster during the Poster Session for discussion.** Full dinner will be available during the poster session (included in the registration fee, advance online registration requested).

The standard size for all posters is 0,85 m x 1,2 m (DIN A 0 – German Standard) vertically oriented. Material to mount the posters will be available at the on-site conference office. It is the presenter’s own responsibility to set-up his/her poster on the assigned poster board and to remove it at the end of the conference. Posters should be hanged up on Friday afternoon between 16:30 and 18:00 and removed at the end of the postersession.

Posters will be reviewed by a jury during the Poster Session on Friday evening. Presentations will be evaluated according to the following criteria:

- Significance and originality of the work
- Quality of the poster presentation
- Outstanding scientific achievement

A total of 8 presentations will be selected to receive the “Best Poster Award” of 150 € each and free admission to the Bunsen-tagung 2018 for the main author.

The **Poster Award Ceremony** will take place during the Closing Ceremony on **Saturday 27 May 2017 at 16:00**.

**Only authors present at the Closing Ceremony will be awarded.**

**KARRIEREFORUM** (in German only)**Thursday, 25 May 2017****11:30 – 14:30**

The Karriereforum (career forum) is an annual symposium organised by the Karriereforum working group of the DBG. It aims at scientists in earlier stages of their careers (between PhD and first appointment as a professor), and provides a forum for discussion of and exchange on career related issues.

The topic of this year’s forum is **“Towards the Professorship – Dos and Donts in Academia”**. The presentation by Mr. Noack (DHV) will give an overview over the German tenure-track system and point out the major pitfalls. Further, within the framework of a podium discussion we will give opportunity to all participants to ask burning questions to our knowledgeable discussants.

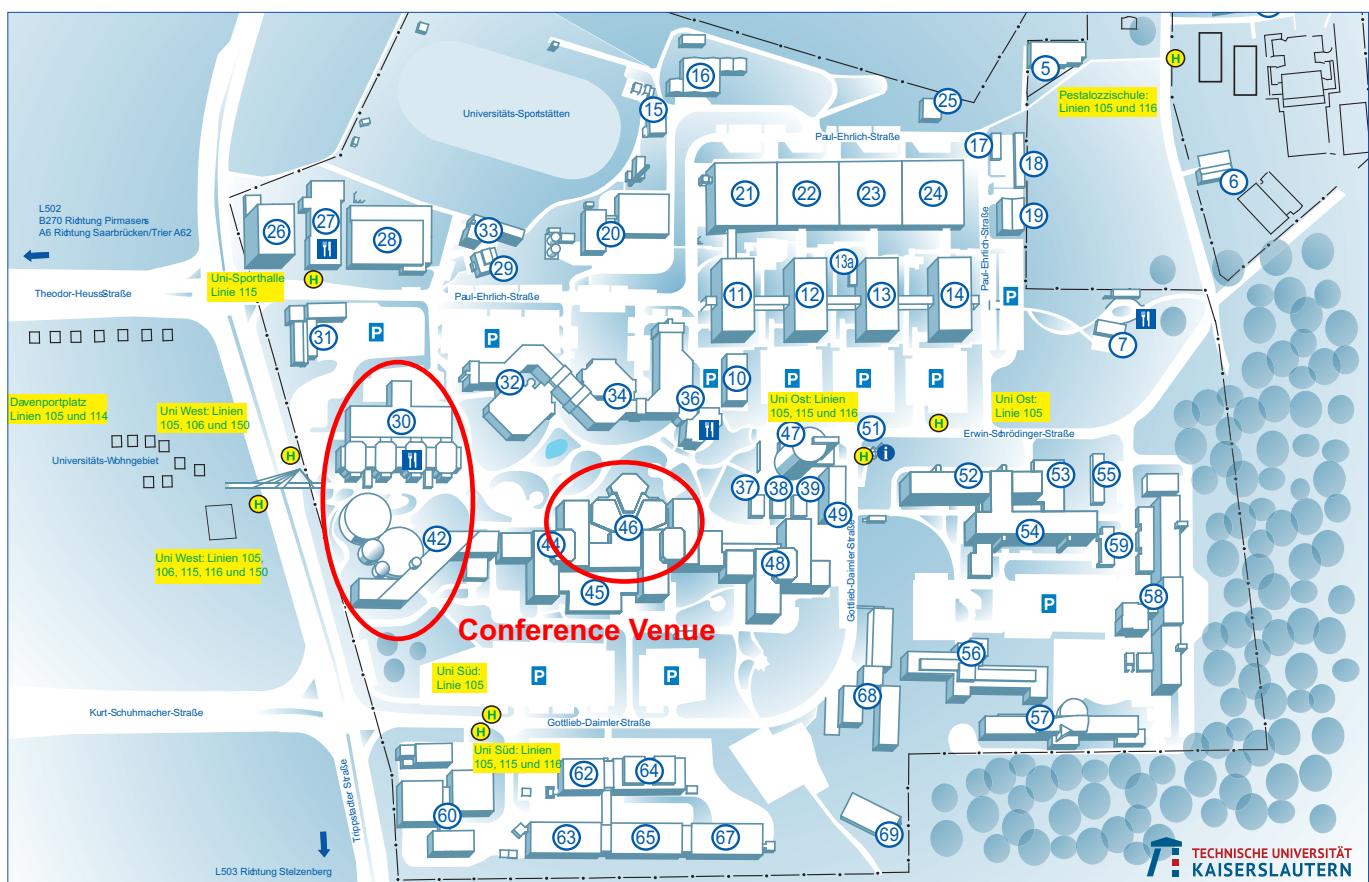
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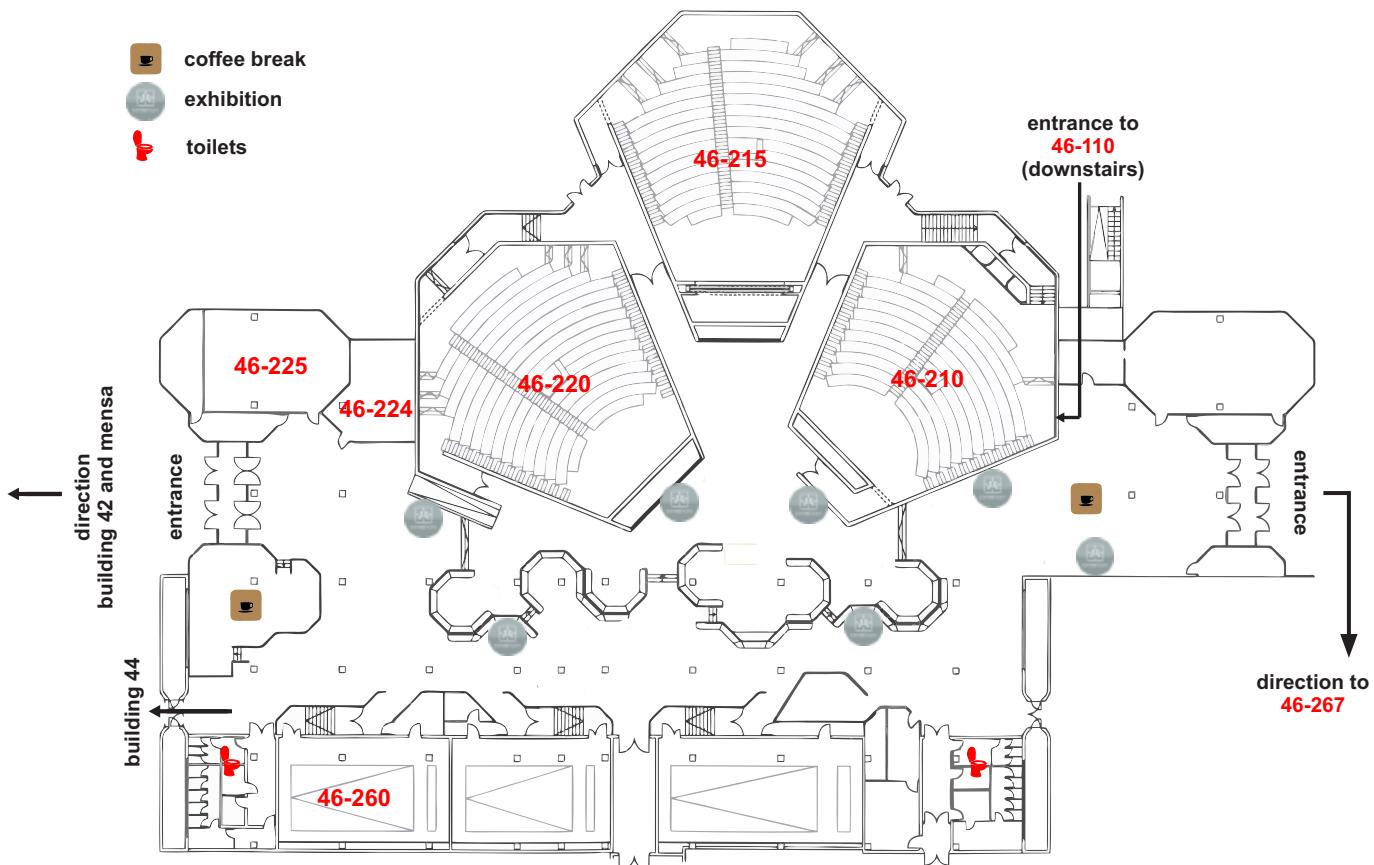
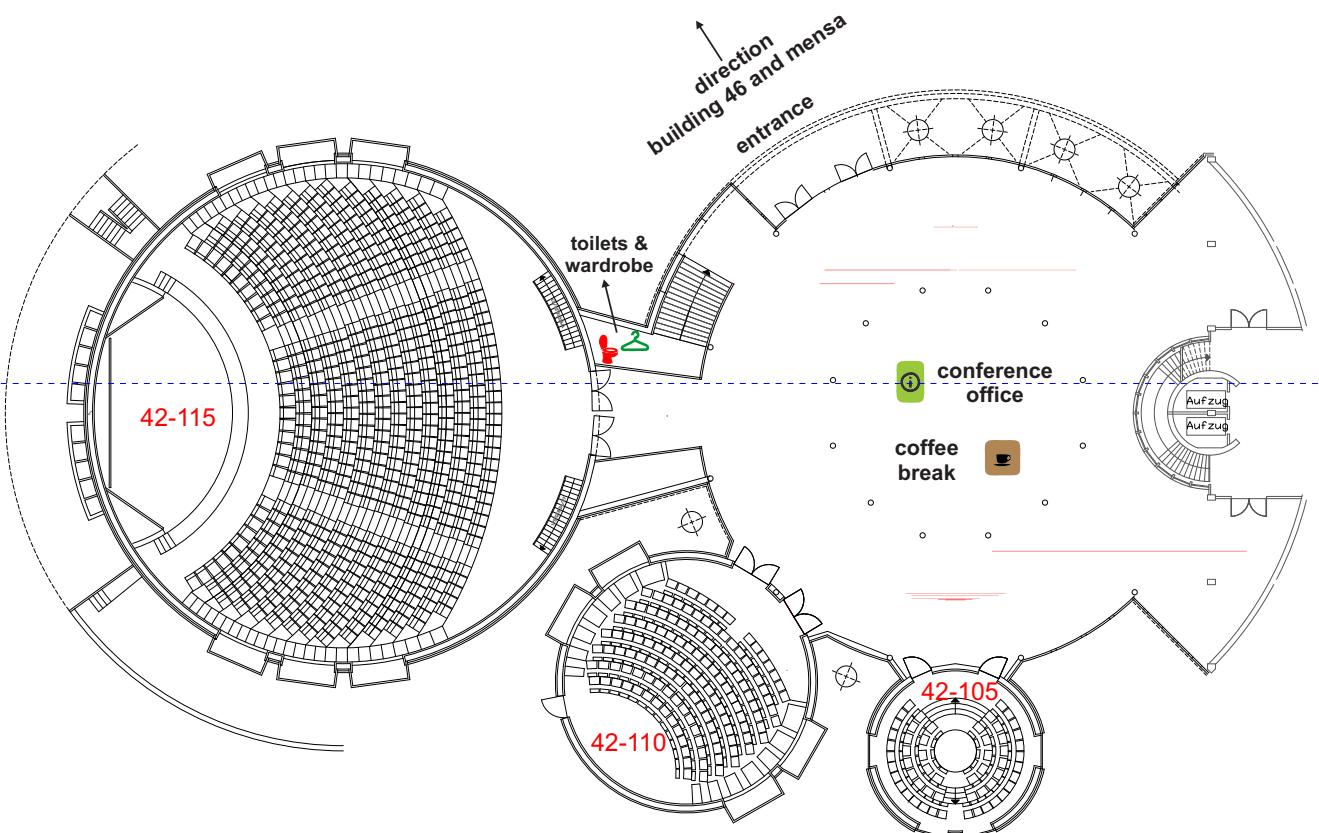
11:30 – 11:35	Eröffnung des Karriereförums
11:35-12:30	<b>Karrierewege in die Professur</b> <b>Sascha-Sven Noack Noack</b> , Deutscher Hochschulverband, Bonn
12:30 – 13:00	Pause mit Kaffee und Brötchen und Netzwerken
13:00 – 14:30	<b>PODIUMSDISKUSSION</b> <b>Weichenstellung für die Professur – Dos and Donts in Academia</b> Prof. Ulrike Woggon, TU Berlin Prof. Klaus Rademann, HU Berlin Prof. Melanie Schnell, MPI Hamburg/Uni Kiel Sascha Noack Deutscher Hochschulverband, Bonn Wolfgang Wachter Deutsche Forschungsgesellschaft, Bonn

More and regularly updated information on the conference is available at

**[www.bunsentagung.de](http://www.bunsentagung.de)**

## MAP



**BUILDING 46****BUILDING 42**



Deutsche Bunsen-Gesellschaft für physikalische Chemie e.V.  
German Bunsen Society for Physical Chemistry  
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60486 Frankfurt am Main/D  
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