

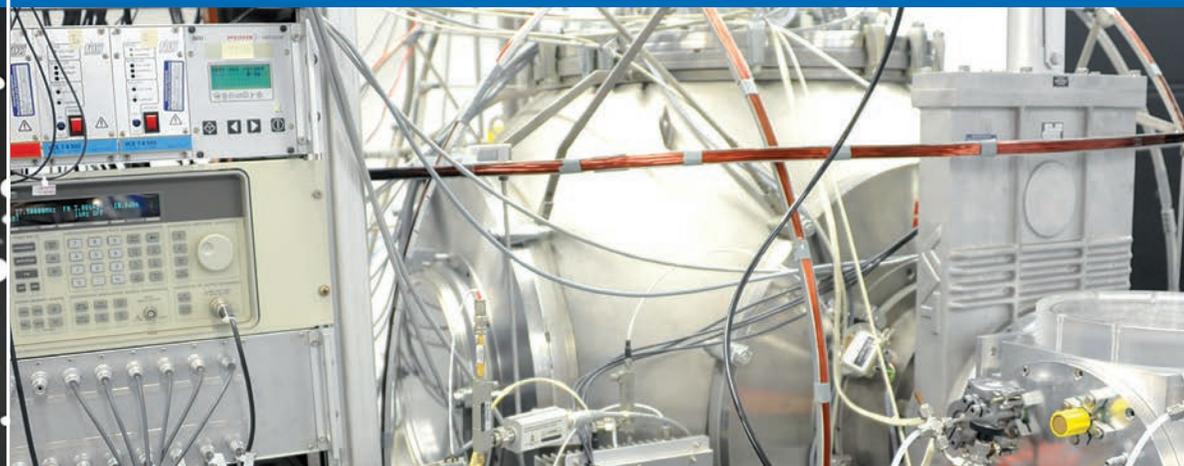


BUNSENTAGUNG 2018

117th General Assembly of the German Bunsen Society for Physical Chemistry

Featuring an industrial symposium with accompanying exhibition
and Karriereforum

10 – 12 May 2018 · Hannover · Germany



PROGRAMME

Kinetics in the Real World

www.bunsentagung.de



11
102
1004

Leibniz
Universität
Hannover

Institut für
Physikalische Chemie
und Elektrochemie



GDCh
GESELLSCHAFT
DEUTSCHER CHEMIKER

CONTENTS

INVITATION	45
COMMITTEES / ORGANISATION	46
EXHIBITION & SPONSORING	47
PROGRAMME AT A GLANCE	48 – 49
OPENING LECTURE / PLENARY LECTURES	50
MEETINGS OF THE GERMAN BUNSEN SOCIETY	51
LECTURE PROGRAMME	51 – 63
Thursday, 10 May 2018	51
Friday, 11 May 2018	52 – 57
Saturday, 12 May 2018	58 – 63
POSTER PROGRAMME	64 – 74
ORAL SESSIONS / PRESENTATION UPLOAD	75
SOCIAL PROGRAMME	76
GENERAL INFORMATION	77 – 80
Registration fees	77
Registration	77
Payment	77
Cancellation	77
Accommodation	77
Venue	78
How to reach the venue	78
Opening hours on-site conference office	78
Contacts	78
Conference languages	78
Child care	78
Internet service	78
Poster session and poster awards	79
yPC-Karriereforum	79
eDu-Forum	79
Map	80

As of 20 February 2018, subject to alterations. Presentation title and authors' information as conveyed by the corresponding author.
Correctness not warranted by the DBG.

MAIN TOPIC:**“Kinetics in the Real World”**

Physical chemistry contributes to all facets of molecular sciences and thus key technologies of the 21st century by enabling analysis of chemical processes on the molecular level. The impact of such experimental and theoretical work can hardly be overestimated. Environmental chemistry, atmospheric processes, climate change, sustainable industrial production, environmentally friendly transportation are just a few of the subjects that have been profiting of the understanding and guidance offered from “Kinetics in the Real World”.

From elementary reactions to complex mechanisms, reaction kinetics is vital to understand and predict the behaviour and development of reactive systems. Progress is being made in experimental techniques to identify reactive intermediates, charge carriers, clusters and nanoscale products even in unusual or hostile environments, in theoretical chemistry to understand the reactivity and the dynamic evolution of the system down to the smallest scales in space and time, and in computer simulation to design and optimize processes and devices or to derive likely scenarios for the future. With this background, the Bunsentagung in Hannover focuses specifically on the insight and guidance that may be expected from understanding fundamental reaction kinetics to address and solve real-world problems. These real-world challenges are omnipresent comprising the broad spectrum of chemical disciplines including atmospheric, environmental, photo- and astrochemistry as well as catalytic processes, kinetics at interfaces and transport in the solid state. They may include energy-related topics such as power generation, transportation, energy storage, biomass conversion, combustion, pyrolysis and gasification, or address processes such as radical polymerisation, plasma processing, chemical vapour deposition, and flame synthesis of functional materials. From a joint perspective on the important contributions to such real-world examples, further synergies are anticipated and will provide perspectives for further developments.

To complement an enormous variety of experimental approaches theoretical studies are highly useful to gain insight into the kinetics of processes of environmental systems and applied processes on the molecular level, thus aiding the interpretation of experimental findings. Scaled to the size of the system, advanced ab initio and DFT-based chemical methods or molecular dynamics simulations are applied; the latter even allowing modelling of large chemical entities.

The concepts and methods in physical chemistry branch out into as many fields of real-world applications as there are quests in chemistry. This meeting should bring together outstanding scientists to discuss leading-edge research, industrial demand and environmental challenges. The synergies of academic and industrial research are far from being exploited and bear great potential to push the frontiers of chemistry faster and further than they could alone. The strong interdisciplinary aspect of the main topic of the Bunsentagung 2018 should foster discussions and spawn new collaborations across the boundaries between scientific exploration and its application or occurrence in the real world.

The Bunsentagung 2018 on “Kinetics in the Real World” in Hannover will provide an excellent platform for fruitful research activities and exchange across disciplines with a focus on the application of physical and theoretical chemistry in research and development. The topic will be highlighted by a suite of distinguished international speakers with forefront international expertise in this field.

COMMITTEE / ORGANISATION

PROGRAMME COMMITTEE

Jörg-August Becker	Hannover/DE	Paul Heitjans	Hannover/DE
Nadja Carola Bigall	Hannover/DE	Klaus-Dieter Hungenberg	Ludwigshafen/DE
Jürgen Caro	Hannover/DE	Ronald Imbihl	Hannover/DE
Johannes Deiglmayr	Zürich/CH	Jürgen Janek	Gießen/DE
Bernhard Dick	Regensburg/DE	Katharina Kohse- Höinghaus	Bielefeld/DE
Dirk Dorfs	Hannover/DE	Jannika Lauth	Delft/NL
Armin Feldhoff	Hannover/DE	Uwe Nickel	Frankfurt (Main)/DE
Gernot Friedrichs	Kiel/DE	Matthias Olzmann	Karlsruhe/DE
Frank Gießelmann	Stuttgart/DE	Rolf Schäfer	Darmstadt/DE
Leticia González	Wien/AT	Jürgen Troe	Göttingen/DE
Jens-Uwe Grabow	Hannover/DE	Karl-Michael Weitzel	Marburg/DE

LOCAL AND SCIENTIFIC ORGANISERS

Jörg-August Becker	Hannover/DE	Irmgard Frank	Hannover/DE
Nadja Bigall	Hannover/DE	Jens-Uwe Grabow	Hannover/DE
Jürgen Caro	Hannover/DE	Paul Heitjans	Hannover/DE
Dirk Dorfs	Hannover/DE	Ronald Imbihl	Hannover/DE
Armin Feldhoff	Hannover/DE	Karl Jug	Hannover/DE

HOST



Deutsche Bunsen-Gesellschaft für physikalische Chemie e.V.
 German Bunsen Society for Physical Chemistry
 Varrentrappstraße 40-42
 60486 Frankfurt am Main/DE
 Phone: +49 69 7917-363
 Fax: +49 69 7917-1363
 E-mail: geschaeftsstelle@bunsen.de
 Internet: www.bunsen.de

Organisational support by:

Gesellschaft Deutscher Chemiker e.V.



Leibniz Universität Hannover



EXHIBITION & SPONSORING

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

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

LIST OF EXHIBITORS

(as of 20 February 2018)

- **academics GmbH**, Hamburg/DE
- **Alexander von Humboldt-Stiftung**, Bonn/DE
- **Belltec Ing. Büro Glocke**, Wesel/DE
- **Bruker Optik GmbH**, Ettlingen/DE
- **COHERENT (Deutschland) GmbH**, Dieburg/DE
- **DFG Deutsche Forschungsgemeinschaft e.V.**, Bonn/DE
- **Newport Spectra-Physics GmbH**, Darmstadt/DE
- **Wiley-VCH**, Weinheim/DE

LIST OF SPONSORS

(as of 20 February 2018)

- **BASF SE**, Ludwigshafen/DE
- **Continental Reifen Deutschland GmbH**, Hannover/DE
- **HCS Holding GmbH**, Königstein/DE
- **PCCP Physical Chemistry Chemical Physics**, Cambridge/UK

FURTHER FINANCIAL SUPPORT

(as of 20 February 2018)

- **Leibniz Universitätsgesellschaft**, Hannover/DE
- **Solvay GmbH**, Hannover/DE

PROGRAMME AT A GLANCE

Thursday, 10 May 2018

11:30-14:30	Institut für Physikalische Chemie und Elektrochemie	eDu-Forum
11:30-14:30		yPC-Forum (Karriere Seminar, in German only)
15:00-16:15	Auditorium Maximum, Welfenschloß	Ordentliche Mitgliederversammlung (for members of the DBG only, in German)
16:30-18:15		OPENING CEREMONY
18:15-19:00		OPENING LECTURE New Developments Coupling Chemistry and Global Climate Change James G. Anderson, Harvard University, Cambridge – Chair: J. Troe
19:30-22:30	Panoramic Lounge, HDI-Arena	WELCOME RECEPTION

Friday, 11 May 2018

08:30-09:10	Audimax-E415	PLENARY LECTURE: Olaf Deutschmann – Chair: K. Kohse-Höinghaus				
	Audimax-E415	Gr. Physik Hörsaal - E214	Hörsaal - E001	Hörsaal - F303	Hörsaal - B305	Hörsaal - B302
	Main Topic	Main Topic Industrial Applications	Photochemistry	Catalysis	Biophysical Chemistry	Energy Conversion and Storage
Chair	K. Kohse-Höinghaus	P. Heltjans	T. Gutmann	M. Schmid	S. Kruss	A. Feldhoff
09:25-09:45	INVITED LECTURE Beuermann	Plass	Naghilou	Hunger	Alahmari	Schepp
09:45-10:05	Janek	Fischer	Vyshnepolyks	Kleber	Ma	Islam
10:05-10:25	Lenzer	INVITED LECTURE Lacayo-Pineda	Paulis	Lunkenbein	Heid	Brummel
10:25-10:45			Lauterbach	Kräuter	Mann	Falkenstein
10:45-11:05	COFFEE BREAK					
	Main Topic	Main Topic Industrial Applications	Photochemistry	Catalysis	Biophysical Chemistry	Transport
Chair	H. Herrmann	B. Abel	N. Bigall	J. Paier	T. Kottke	A. R. Genreith-Schriever
11:05-11:25	INVITED LECTURE Carpenter	Tracht	Maus	Sterrer	Habercorn	Schäfer
11:25-11:45	Hoffmann	Rabbow	Kus	Mohrhusen	Simmchen	Düvel
11:45-12:05	Zeuch	INVITED LECTURE Votsmeier	Novelli	Hess	Neubert	Draber
12:05-12:25			Oncak	Werner	Garidel	Yang
12:25-13:25	LUNCH BREAK					
13:25-14:05	Audimax-E415	PLENARY LECTURE: William H. Green – Chair: G. Friedrichs				
	Audimax-E415	Gr. Physik Hörsaal - E214	Hörsaal - E001	Hörsaal - F303	Hörsaal - B305	Hörsaal - B302
	Award Winners	Main Topic Industrial Applications	Photochemistry	Chemical Dynamics and Kinetics	Molecular Structure and Dynamics	Thermodynamics/ Extraterrestrial Chemistry
Chair	U. Nickel	J. Wullenkord	T. Lenzer	M. Braun-Unkhoff	M. Gerhards	J.-A. Becker
14:20-14:40	Ewald-Wicke	INVITED LECTURE Deglmann	Johny	Bastian	Domingos	Mascotto
14:40-15:00	Paul Bunge	Lade	Geissler	Fittschen	Müller-Werkmeister	Mezger
15:00-15:20	Nernst-Haber- Bodenstein I	Vale	Kutta	Sölter	Schmitt	Stuckenholtz
15:20-15:40	Nernst-Haber- Bodenstein II	Bachmann	Stellmacher	Schaefer	Debnath	Wittenberg
15:40-16:00	DFG/AvH Wachter/Hoffmann	Straub	Hemberger	Obenchain	Chatterjee	
16:00-16:20	COFFEE BREAK					
	Main Topic	Main Topic Industrial Applications	Hot Topic	Chemical Dynamics and Kinetics	Molecular Structure and Dynamics	Electrochemistry
Chair	T. Zeuch	B. Atakan	E. Rühl	M. Schnell	J. Küpper	J. Janek
16:20-16:40	INVITED LECTURE Glarborg	Wocke	Mom	Seher	Gleim	Vargas-Barbosa
16:40-17:00	Ruwe	Torkashvand	Hausbrand	Kahnt	Roemelt	Hofmann
17:00-17:20	Shu	Börger	Lippe	Riedinger	Fuchs	Müller
17:20-17:40	Kasper	INVITED LECTURE Recker	Meyer	Peukert	Wiese	Lorger
17:40-18:00			Parras	Klemmed	Schwing	Genreith-Schriever
18:00-19:30	Galerie, Welfenschloß	POSTER EVENING (even numbers)				
19:30-21:00		POSTER EVENING (odd numbers)				

Saturday, 12 May 2018

08:30-09:15	Audimax-E415	PLENARY LECTURE: Sotiris E. Pratsinis – <i>Chair: M. Olzmann</i>				
	Audimax-E415	Gr. Physik Hörsaal - E214	Hörsaal - E001	Hörsaal - F303	Hörsaal - B305	Hörsaal - B302
	Main Topic	Main Topic	Photochemistry	Chemical Dynamics and Kinetics	Molecular Structure and Dynamics	Electrochemistry
<i>Chair</i>	<i>M. Olzmann</i>	<i>M. Suhm</i>	<i>K. Boldt</i>	<i>C. Fittschen</i>	<i>J. Deiglmayr</i>	<i>J.P. Hofmann</i>
09:25-09:45	INVITED LECTURE	von Boehn	Wächtler	Klocke	Yachmenev	Alshalfouh
09:45-10:05	König	Giehr	Rosebrock	Krüger	Neumann	Oezaslan
10:05-10:25	Burek	INVITED LECTURE	Himstedt	Hesse	Pramann	Wang
10:25-10:45	Pelucchi		Maier	Lauth	Richter	Klee
10:45-11:05	COFFEE BREAK					
	Main Topic	Main Topic	Photochemistry	Chemical Dynamics and Kinetics	Hot Topic	Energy Conversion and Storage
<i>Chair</i>	<i>R. Imbihl</i>	<i>K. A. Heufer</i>	<i>D. Dorfs</i>	<i>P. Hemberger</i>	<i>B. Dietzek</i>	<i>K.-M. Weitzel</i>
11:05-11:25	INVITED LECTURE	van der Linde	Rusch	Jacobs	Stuhr	Chen
11:25-11:45	Schauermann	Haynes	Tietze	Methling	Wendt	Marschall
11:45-12:05	Schaube	INVITED LECTURE	Heinke	Piccini	Lesarri	Indris
12:05-12:25	Gossler		Schulz	Eichler	Gerke	Schleier
12:25-13:25	LUNCH BREAK					
13:25-14:05	Audimax-E415	PLENARY LECTURE: Paola Caselli – <i>Chair: J.-U. Grabow</i>				
	Audimax-E415	Gr. Physik Hörsaal - E214	Hörsaal - E001	Hörsaal - F303	Hörsaal - B305	Hörsaal - B302
	Main Topic	Main Topic	Photochemistry	Catalysis	Biophysical Chemistry	Transport
<i>Chair</i>	<i>J. Caro</i>	<i>G. Friedrichs</i>	<i>J. Lauth</i>	<i>S. Tschierlei</i>	<i>A. Lesarri</i>	<i>G. Niedner-Schattebrug</i>
14:20-14:40	Kraus	Brandl	Kautek	Paier	Wiebeler	Scheele
14:40-15:00	Borodin	Atakan	Schröder	Siemer	Dreier	Niedermaier
15:00-15:20	Feldt	Weber	Hoberg	Alessio	Das	Schmid
15:20-15:40	Thissen	Wullenkord	Falcon Casas	Baldofski	Möller	Boldt
15:55-16:25	Audimax-E415	Poster Awards and Closing Ceremony				

OPENING LECTURE / PLENARY LECTURES

OPENING LECTURE

Thursday, 10 May 2018

- 18:15 – 19:00 **New Developments Coupling Chemistry and Global Climate Change**
James G. Anderson, Harvard University, Cambridge/US

PLENARY LECTURES

Friday, 11 May 2018

- 08:30 – 09:10 **Reaction mechanisms for power generation, transportation and energy storage**
Olaf Deutschmann, Karlsruher Institut für Technology, Karlsruhe/DE
- 13:25 – 13:45 **Predicting the Anti-Knock Performance of Fuel Additives with Kinetics**
William H. Green, Massachusetts Institute of Technology, Cambridge/US

Saturday, 12 May 2018

- 08:30 – 09:15 **Flame-made Materials: from Carbon Black to Breath Analysis Sensors**
Sotiris E. Pratsinis, ETH, Zurich/CH
- 13:25 – 14:05 **The first steps toward pre-biotic molecules at the dawn of star and planet formation**
Paola Caselli, MPI for Extraterrestrial Physics, Garching/DE

MEETINGS OF THE GERMAN BUNSEN SOCIETY

Thursday, 10 May 2018

08:00 – 10:00	Vorstandssitzung* (on invitation only)	Room 115/2504
09:00 – 10:30	Sitzung der Themenkommission*	Room 115/2504
10:30 – 12:30	Sitzung des Ständigen Ausschusses* (on invitation only)	Room 115/2504
11:30 – 14:30	eDu-Forum*	Room 010/2504
11:30 – 14:30	yPC- Karriereforum*	Room 007/2504
14:30 – 15:00	Sitzung der Studienkommission*	Room 010/2504
15:00 – 16:15	Ordentliche Mitgliederversammlung* (for members of the DBG only)	Audimax

Friday, 11 May 2018

12:25 – 13:25	Seminar Wiley-VCH	Room B305
12:25 – 13:25	Seminar Academics	Room B302
12:25 – 13:25	Women's networking lunch (registration required)	Room 115/2504
21:30	yPC Networking evening	Kuriosum

Saturday, 12 May 2018

12:25 – 13:25	yPC Mitgliederversammlung* (for members of the yPC only)	Room 115/2504
---------------	---	---------------

* in German only

LECTURE PROGRAMME

Thursday, 10 May 2018

	Institut für Physikalische Chemie und Elektrochemie
11:30 – 14:30	eDu-Forum
11:30 – 14:30	yPC-Forum (Karriere Seminar, in German only)
	Auditorium Maximum, Welfenschloß
15:00 – 16:15	Ordentliche Mitgliederversammlung (for members of the DBG only, in German)
16:30 – 18:15	OPENING CEREMONY
18:15 – 19:00	OPENING LECTURE New Developments Coupling Chemistry and Global Climate Change James G. Anderson, Harvard University, Cambridge – <i>Chair: J. Troe</i>
	Panoramic Lounge, HDI-Arena
19:30 – 22:30	WELCOME RECEPTION

LECTURE PROGRAMME

Friday, 11 May 2018

Morning

Audimax – E415		Großer Physik-Hörsaal – E214	
Chair: K. Kohse-Höinghaus		Chair: P. Heitjans	
Main Topic	Main Topic	Industrial Application	
08:30		08:30	
PLENARY LECTURE Reaction mechanisms for power generation, transportation and energy storage O. Deutschmann, Karlsruhe/DE			
09:25		09:25	
INVITED LECTURE Detailed kinetics of radical polymerizations studied via pulsed-laser initiated polymerizations and modeling S. Beuermann, Clausthal-Zellerfeld/DE	Fundamental Analytical Assessment of the degradation of Polyalkylene Glycols as Lubricantss in Turbo-Machinery M. Plass, Horgen/CH, M. Greaves, Horgen/CH		
09:45		Determination of fast curing epoxy matrix materials for high volume car application F. Fischer, Wolfsburg/DE, R. Thomas, Wolfsburg/DE, F. Horn, Wolfsburg/DE, F. Wehler, Wolfsburg/DE	09:45
10:05	Kinetics and Mechanisms of Electrolyte Degradation in Lithium (ion) Batteries J. Janek, Gießen/DE, T. Brezesinski, Eggenstein-Leopoldshafen/DE, J. Sann, Gießen/DE	INVITED LECTURE Innovative Kinetic Approaches in Rubber Technology J. Lacayo, Hannover/DE, J. Schawe, Greiffensee/CH, T. Rauschmann, Wetzlar/DE	10:05
10:25	Exciton and coherent phonon dynamics in BiI₃ and the metal-deficient vacancy-ordered perovskite (CH₃NH₃)₃Sb₂I₉ T. Lenzer, Siegen/DE, M. Scholz, Siegen/DE, M. Morgenroth, Siegen/DE, K. Oum, Siegen/DE		10:25
10:45		10:45	
COFFEE BREAK			
Audimax – E415		Großer Physik-Hörsaal – E214	
Chair: H. Herrmann		Chair: B. Abel	
Main Topic	Main Topic	Industrial Application	
11:05		11:05	
INVITED LECTURE Kinetics at the ocean interface: Ozone deposition and iodine emission L. Carpenter, York/GB, R. Chance, York/GB, L. Tinel, York/GB, M. Shaw, York/GB, A. Saint, York/GB, D. Loades, York/GB, T. Sherwen, York/GB, M. J. Evans, York/GB, S. Ball, Leicester/GB, T. Adams, Leicester/GB	Contributions from Kinetic Studies to the Development of a New Rubber Production Process U. Tracht, Köln/DE		
11:25		Physical Chemistry of Thermal Activation and Electrochemical Reactivity of Carbon Felts T. J. Rabbow, Vienna/AT	11:25
11:45	Oxidation of substituted aromatic hydrocarbons in the tropospheric aqueous phase: Kinetic mechanism development and modelling E. H. Hoffmann, Leipzig/DE, A. Tilgner, Leipzig/DE, R. Wolke, Leipzig/DE, H. Herrmann, Leipzig/DE	INVITED LECTURE Surface Kinetics in the Real World: Modelling Industrial Catalytic Reactors, and why it is more difficult than we thought 15 years ago M. Votsmeier, Hanau/DE	11:45
12:05	Aggregation kinetics in supersaturated H₂SO₄ vapour T. Zeuch, Göttingen/DE, P. T. M. Carlsson, Göttingen/DE		12:05
12:25		12:25	
LUNCH BREAK			

Friday, 11 May 2018		Morning	
Audimax – E415			
<i>Chair: K. Kohse-Höinghaus</i>			
08:30	PLENARY LECTURE Reaction mechanisms for power generation, transportation and energy storage O. Deutschmann, Karlsruhe/DE	08:30	
Hörsaal – E001		Hörsaal – F303	
Photochemistry		Catalysis	
<i>Chair: T. Gutmann</i>		<i>Chair: M. Schmid</i>	
09:25	Femtosecond laser generation of microbumps on stacked Cu/Ag thin films A. Naghilou, Vienna/AT, O. Armbruster, Vienna/AT, J. Schubert, Vienna/AT, L. Zhigilei, Charlottesville/US, W. Kautek, Vienna/AT	Association of phosphoric acid organo-catalysts with imines J. Hunger, Mainz/DE, C. Malm, Mainz/DE, H. Kim, Mainz/DE, M. Wagner, Mainz/DE	09:25
09:45	Non-linear laser-induced surface structuring far below the melting threshold M. Vyshnepolsky, Bochum/DE, N. Osterloh, Bochum/DE, T. Pan, Bochum/DE, C. Zaum, Hannover/DE, K. Morgenstern, Bochum/DE	Inline Infrared Spectroscopic Concentration Determination in a Solvent-free Biocatalytic Reactive Rectification J. Kleber, Hamburg/DE, M.-A. Christlieb, S. Kühn, B. Wind, A. Stöbener, I. Smirnova, A. Liese, Hamburg/DE	09:45
10:05	Laser-induced breakdown spectroscopy of metal coatings: Influence of laser wavelength E. Paulis, Vienna/AT, U. Pacher, Vienna/AT, S. Dinu, Bucharest/RO, T. Nagy, Vienna/AT, R. Rădvan, Bucharest/RO, W. Kautek, Vienna/AT	Unraveling the Structural Complexity of Orthorhombic (Mo,V)O_x by Transmission Electron Microscopy T. Lunkenbein, Berlin/DE, L. Masliuk, Berlin/DE, A. Trunschke, Berlin/DE, M. G. Willinger, Berlin/DE, R. Schlögl, Berlin/DE	10:05
10:25	Fast Polymerization of Slowly Propagating Monomers via Iniferter RAFT Polymerization in Continuous Micro- and Milli-Flow Reactors F. Lauterbach, Hamburg/DE, M. Rubens, Melbourne/AU, T. Junkers, Melbourne/AU, V. Abetz, Hamburg/DE	Bulk Defect Dependent Adsorption of Acetone on Rutile TiO₂(110) J. Kräuter, Oldenburg/DE, K. Al-Shamery, Oldenburg/DE	10:25
10:45	COFFEE BREAK		10:45
Hörsaal – E001		Hörsaal – F303	
Photochemistry		Catalysis	
<i>Chair: N. Bigall</i>		<i>Chair: J. Paier</i>	
11:05	Search for Stronger Super-Photoacids D. Maus, Saarbrücken/DE, A. Grandjean, Saarbrücken/DE, G. Jung, Saarbrücken/DE	Charge Transfer and Orbital Level Alignment at Inorganic/Organic Interfaces - The Role of Dielectric Interlayers M. Sterrer, Graz/AT, M. Hollerer, Graz/AT, P. Hurdax, Graz/AT, D. Lüftner, Graz/AT, P. Puschnig, Graz/AT, G. Koller, Graz/AT, M. Ramsey, Graz/AT	11:05
11:25	Long-lived coherences in perfluorinated aromatic compounds as a probe of $\pi\pi^*$ – $\pi\sigma^*$ vibronic coupling J. A. Kus, Kiel/DE, O. Hüter, Kiel/DE	Defect density dependence of partial oxidation and deoxygenation reactions of small organic compounds on rutile TiO₂ (110) surfaces L. Mohrhusen, Oldenburg/DE, M. Osmić, Oldenburg/DE, K. Al-Shamery, Oldenburg/DE	11:25
11:45	Giant Terahertz Kerr effect in water F. Novelli, Bochum/DE, F. Sebastiani, Bochum/DE, C. Hoberg, Bochum/DE, N. Stavrias, Nijmegen/NL, A. F. G. Van Der Meer, Nijmegen/NL, G. Schwaab, Bochum/DE, M. Havenith, Bochum/DE	Monitoring defect and adsorbate dynamics in supported gold catalysts using combined <i>operando</i> spectroscopy C. Hess, Darmstadt/DE, C. Schilling, Darmstadt/DE	11:45
12:05	Photochemical Changes Induced by Molecular Environment: Experimental-Theoretical Investigations on Small Ionic Systems M. Oncak, Innsbruck/AT, T. Taxer, Innsbruck/AT, N. Bersenkowitsch, Innsbruck/AT, D. Muß, Innsbruck/AT, C. van der Linde, Innsbruck/AT, M. K. Beyer, Innsbruck/AT	How O Vacancies influence the Interaction of H₂ with CeO₂(111) K. Werner, Berlin/DE, X. Weng, Berlin/DE, F. Calaza, Santa Fe/AR, M. Sterrer, Graz/AT, T. Kropp, Berlin/DE, J. Paier, Berlin/DE, J. Sauer, Berlin/DE, M. Wilde, Tokyo/JP, K. Fukutani, Tokyo/JP, S. Shaikhutdinov, Berlin/DE, H.-J. Freund, Berlin/DE	12:05
12:25	LUNCH BREAK		12:25

LECTURE PROGRAMME

Friday, 11 May 2018

Morning

Audimax – E415			
Chair: K. Kohse-Höinghaus			
08:30	PLENARY LECTURE Reaction mechanisms for power generation, transportation and energy storage O. Deutschmann, Karlsruhe/DE	08:30	
Hörsaal – B305	Hörsaal – B302		
Biophysical Chemistry	Energy Conversion and Storage		
Chair: S. Kruss		Chair: A. Feldhoff	
09:25	Trace gas analysis by diode laser photoacoustic spectroscopy in a Helmholtz resonator for environmental and biological applications S. Alahmari, Sheffield/GB, M. Hippler, Sheffield/GB	A thermodynamic description of the battery material LiCoO₂ based on ionic and electronic work functions J. Schepp, Marburg/DE, S. Schuld, Marburg/DE, R. Hausbrand, Darmstadt/DE, M. Fingerle, Darmstadt/DE, W. Jägermann, Darmstadt/DE, K.-M. Weitzel, Marburg/DE	09:25
09:45	Characterisation of the ion atmosphere around DNA by THz spectroscopy C. Y. Ma, Bochum/DE, M. Gebala, Stanford/US, D. Herschlag, Stanford/US, G. Schwaab, Bochum/DE, M. Havenith, Bochum/DE	Investigation of Ion Diffusion in Solid State Materials for Energy Storage: Insights from Theory M. Islam, Bonn/DE, P. Heitjans, Hannover/DE, T. Bredow, Bonn/DE	09:45
10:05	Linear response theory in solvation dynamics – A critique E. Heid, Vienna/AT, W. Moser, Vienna/AT, C. Unterberger, Vienna/AT, C. Schröder, Vienna/AT	Electrochemically Controlled Solar Energy Storage in Strained Organic Molecules: In-Situ Spectroscopy in the Norbornadiene-Quadracyclane System O. Brummel, Erlangen/DE, F. Waidhas, Erlangen/DE, M. Jevric, Gothenburg/SE, U. Bauer, Erlangen/DE, Y. Wu, Erlangen/DE, S. Bochmann, Erlangen/DE, T. Döpfer, Erlangen/DE, A. Görling, Erlangen/DE, C. Papp, Erlangen/DE, J. Bachmann, Erlangen/DE, K. Moth-Poulsen, Gothenburg/SE, J. Libuda, Erlangen/DE	10:05
10:25	Peptide-barrel encapsulated carbon nanotubes F. A. Mann, Göttingen/DE, J. Horlebein, Göttingen/DE, F. Thomas, Göttingen/DE, S. Kruss, Göttingen/DE	Transport Kinetics of Proton Conductors by means of ECR A. Falkenstein, Aachen/DE, M. Martin, Aachen/DE	10:25
10:45	COFFEE BREAK		10:45
Hörsaal – B305	Hörsaal – B302		
Biophysical Chemistry	Transport		
Chair: T. Kottke		Chair: A. R. Genreith-Schriever	
11:05	Quantum Dot Based FRET Sensors for Biomedical Applications L. Habercorn, Hamburg/DE, M. Janschel, Hamburg/DE, H. Weller, Hamburg/DE	Site energy distributions in ion conducting glasses M. Schäfer, Marburg/DE, K.-M. Weitzel, Marburg/DE	11:05
11:25	Interactions of biological and artificial microswimmers with microscale objects J. Simmchen, Dresden/DE, J. Bastos, Dresden/DE, A. Revilla, Dresden/DE	Fast ion conduction caused by geometric frustration: Ba_{1-x}Ca_xF₂ A. Düvel, Canterbury/GB, P. Heitjans, Hannover/DE, D. C. Sayle, Canterbury/GB	11:25
11:45	Entropic DNA swelling drives complex cellular behavior E. Neubert, Göttingen/DE, D. Meyer, Göttingen/DE, F. Rocca, Göttingen/DE, A. Kwaczala-Tessmann, Göttingen/DE, S. Senger-Sander, Göttingen/DE, J. Grandke, Göttingen/DE, C. Geisler, Göttingen/DE, A. Egner, Göttingen/DE, M. P. Schön, Göttingen/DE, L. Erpenbeck, Göttingen/DE, S. Kruss, Göttingen/DE	Ion conductivity in doped BaZrO₃ F. M. Draber, Aachen/DE, M. Martin, Aachen/DE	11:45
12:05	Highly Concentrated Therapeutic Protein Solutions – When Protein Systems Become Crowded P. Garidel, Halle (Saale)/DE, J. Hartl, Biberach/DE, M. Blech, Biberach/DE, D. Johannsmann, Clausthal Zellerfeld/DE, D. Hinderberger, Halle (Saale)/DE, P. Garidel, Halle (Saale)/DE	Water Transport Through Carbon Nanomembranes: Combine Exceptionally High Permeance with High Selectivity Y. Yang, Bielefeld/DE, P. Dementyev, Bielefeld/DE, N. Biere, Bielefeld/DE, D. Emmrich, Bielefeld/DE, P. Stohmann, Bielefeld/DE, R. Korzetz, Bielefeld/DE, X. Zhang, Bielefeld/DE, A. Beyer, Bielefeld/DE, S. Koch, Bielefeld/DE, D. Anselmetti, Bielefeld/DE, A. Götzhäuser, Bielefeld/DE	12:05
12:25	LUNCH BREAK		12:25

Friday, 11 May 2018

Afternoon

Audimax – E415		Großer Physik-Hörsaal – E214	
Chair: G. Friedrichs			
13:25	PLENARY LECTURE Predicting the Anti-Knock Performance of Fuel Additives with Kinetics W. H. Green, Cambridge/US	13:25	
Audimax – E415		Großer Physik-Hörsaal – E214	
Award Winners		Main Topic Industrial Application	
Chair: U. Nickel		Chair: J. Wullenkord	
14:20	Ewald Wicke	INVITED LECTURE Prediction of Polymerization Kinetics via Quantum Chemistry P. Deglmann, Ludwigshafen/DE	14:20
14:40	Paul Bunge		14:40
15:00	Nernst-Haber-Bodenstein I	Kinetics in Industry: Applying a toolset from “old school” approaches to digitalization O. Lade, Frankfurt (Main)/DE, E. Akgün, Gendorf/DE, J. Appel, Gendorf/DE, O. Wachsen, Frankfurt (Main)/DE	15:00
15:20	Nernst-Haber-Bodenstein II	Applied Polymerization Kinetics: An Industrial Perspective H. Vale, Ludwigshafen/DE, A. Daiss, Ludwigshafen/DE, W. Gerlinger, Ludwigshafen/DE	15:20
15:40	DFG/AvH, Wachter/Hoffmann	Identification of Kinetics in Multi-Component Systems R. Bachmann, Leverkusen/DE	15:40
16:00	COFFEE BREAK		16:00
Audimax – E415		Großer Physik-Hörsaal – E214	
Main Topic		Main Topic Industrial Application	
Chair: T. Zeuch		Chair: B. Atakan	
16:20	INVITED LECTURE Towards fuel-switching in Diesel engines: High pressure oxidation of simpler hydrocarbons and alcohols P. Glarborg, Lyngby/DK	Modelling the Composite Pultrusion Process by Finite Elements using the Curing Kinetics of a 2K Resin System. C. Wocke, Horgen/CH, M. Siddiqui, Horgen/CH, M. Plass, Horgen/CH, G. Bramante, Corregio/IT, J. Claracq, Terneuzen/NL	16:20
16:40		Modeling of chemistry and mass transfer in a monolithic reactor with sinusoidal channel for the catalytic oxidation of formaldehyde B. Torkashvand, Karlsruhe/DE, T. Schedlbauer, Karlsruhe/DE, M. Casapu, Karlsruhe/DE, J.-D. Grunwaldt, Karlsruhe/DE, O. Deutschmann, Karlsruhe/DE	16:40
17:00	Towards formation of small aromatic compounds: Mass spectrometric investigation of fuel-specific decomposition and growth pathways in selected alkane and alkene flames L. Ruwe, Bielefeld/DE, L. Cai, Aachen/DE, K. Moshhammer, Braunschweig/DE, N. Hansen, Livermore/US, H. Pitsch, Aachen/DE, K. Kohse-Höinghaus, Bielefeld/DE	Thermal Run-away in Lithium-Ion Batteries: Standardisation and Homologation Aspects A. Börger, Wolfsburg/DE	17:00
17:20	Understanding the chemical kinetic details of ammonia oxidation for its optimized use in clean transportation systems B. Shu, Braunschweig/DE, S. K. Vallabhuni, Braunschweig/DE, X. He, Braunschweig/DE, G. Issayev, Thuwal/SA, K. Moshhammer, Braunschweig/DE, A. Farooq, Thuwal/SA, R. X. Fernandes, Braunschweig/DE	INVITED LECTURE Kinetics in Tire Materials Technology C. Recker, Hannover/DE	17:20
17:40	A PEPICO study of key reaction steps in toluene combustion T. Kasper, Duisburg/DE, S. Kluge, Duisburg/DE, T. Bierkandt, Duisburg/DE, P. Hemberger, Villigen/CH, D. Krüger, Stuttgart/DE, P. Oßwald, Stuttgart/DE, M. Köhler, Stuttgart/DE		17:40
18:00	POSTER EVENING (even numbers)		18:00
19:30	POSTER EVENING (odd numbers) (19:30 – 21:00)		19:30
21:30	yPC Networking Evening		21:30

LECTURE PROGRAMME

Friday, 11 May 2018

Afternoon

Audimax – E415			
Chair: G. Friedrichs			
13:25	PLENARY LECTURE Predicting the Anti-Knock Performance of Fuel Additives with Kinetics W. H. Green, Cambridge/US	13:25	
Hörsaal – E001	Hörsaal – F303		
Photochemistry	Chemical Dynamics and Kinetics		
Chair: T. Lenzer	Chair: M. Braun-Unkhoff		
14:20	Hydrogen bond dissociation dynamics of indole-water clusters M. Johnny, Hamburg/DE, T. Kierspel, Hamburg/DE, J. Wiese, J. Onvlee, H. Bieker, T. Mullins, A. Trabattoni, R. Livingstone, Hamburg/DE, G. Coslovich, S. Moeller, J. Aldrich, Menlo Park/US, S. Trippel, J. Küpper, Hamburg/DE	Anionic carbon chain elongation with acetylene B. Bastian, Innsbruck/AT, T. Michaelsen, Innsbruck/AT, J. Meyer, Innsbruck/AT, R. Wester, Innsbruck/AT	14:20
14:40	Tracing the Photodynamics of the Molecular Rotor Thioflavin T in Solution and during Insulin Fibrillization B. Geissler, Bochum/DE, K. Artmann, Bochum/DE, D. Wesberg, Bochum/DE, P. Nuernberger, Bochum/DE	The Reaction of Fluorine Atoms with Methanol: Yield of CH₃O / CH₂OH and Rate Constants of the Reactions CH₃O + CH₃O and CH₃O + HO₂ C. Fittschen, Lille/FR, E. Assaf, Lille/FR, C. Schoemaeker, Lille/FR	14:40
15:00	Stepwise Hydride Transfer in a Biological System: Insights into the Reaction Mechanism of the Light-Dependent Protochlorophyllide Oxidoreductase R. J. Kutta, Regensburg/DE, N. Archipowa, Manchester/GB, D. J. Heyes, Manchester/GB, N. S. Scrutton, Manchester/GB	Experimental and Modelling Study of the Multichannel Thermal Dissociations of CH₃F and CH₂F L. Sölter, Göttingen/DE, C. J. Cobos, La Plata/AR, G. Knight, Clevedon/GB, E. Tellbach, Göttingen/DE, J., Göttingen/DE	15:00
15:20	Dynamics of acetylacetone upon S₂ (¹ππ[*]) photoexcitation by femtosecond time-resolved vibrational absorption spectroscopy R. Stellmacher, Kiel/DE, B. Alves Morais, Kiel/DE, H. Böhnke, Kiel/DE, S. Schatz, Kiel/DE, F. Temps, Kiel/DE	OH radical reactions with oxygenated organic compounds in aqueous solution: A laser flash photolysis investigation T. Schaefer, Leipzig/DE, H. Herrmann, Leipzig/DE	15:20
15:40	Unraveling the primary photochemical processes of the ferrioxalate actinometer S. Straub, Bonn/DE, P. Brünker, Bonn/DE, J. Lindner, Bonn/DE, P. Vöhringer, Bonn/DE	On the Photoelectron Spectrum and Energetics of the meta-Xylylene Diradical P. Hemberger, Villigen PSI/CH, M. Steglich, Villigen PSI/CH, A. Bodi, Villigen PSI/CH, V. B. F. Custodis, Zürich/CH, A. J. Trevitt, Wollongong/AU, G. da Silva, Melbourne/AU	15:40
COFFEE BREAK		16:00	
Hörsaal – E001	Hörsaal – F303		
Hot Topic	Chemical Dynamics and Kinetics		
Chair: E. Rühl	Chair: M. Schnell		
16:20	Electrochemical XPS using confined electrolyte and graphene windows: the case of Pt oxidation R. V. Mom, Berlin/DE, L. Frevel, Berlin/DE, J. J. Velasco Velez, Berlin/DE, A. Knop-Gericke, Berlin/DE, R. Schlögl, Berlin/DE	From Clusters to Nanocrystals: Growth of CdSe Nanocrystals via Magic-Sized Cluster Intermediates R. Seher, Hamburg/DE, C. Palencia Ramirez, Hamburg/DE, F. Lehmkuhler, Hamburg/DE, H. Weller, Hamburg/DE	16:20
16:40	Recent insights on reaction mechanisms at Li-ion electrode-electrolyte interfaces obtained by model experiments R. Hausbrand, Darmstadt/DE, M. Fingerle, Darmstadt/DE, T. Späth, Darmstadt/DE, N. Schulz, Darmstadt/DE	Radiation Chemical GO Reduction – Kinetics and Mechanisms A. Kahnt, Erlangen/DE, S. Eigler, Berlin/DE, R. Fluynt, Leipzig/DE, S. Naumov, Leipzig/DE, B. Abel, Leipzig/DE	16:40
17:00	Direct observation of cluster size distributions during nucleation in pulsed Laval expansions M. Lippe, Zürich/CH, S. Chakrabarty, Zürich/CH, J. J. Ferreira, Zürich/CH, R. Signorell, Zürich/CH	Kinetic Growth Instabilities in Isotropic Materials Lead to Nanoplatelets A. Riedinger, Mainz/DE, F. D. Ott, Mainz/DE, P. N. Knüsel, Mainz/DE, S. C. Erwin, Mainz/DE, D. J. Norris, Mainz/DE	17:00
17:20	Examining the Dynamics in Supersonic Expansions: An FTIR Imaging Study of Cluster Formation and Decomposition in Shock Waves K. A. E. Meyer, Göttingen/DE, M. A. Suhm, Göttingen/DE	High temperature gas-phase-kinetics of tetramethoxysilane decomposition and its bimolecular reaction with H atoms S. Peukert, Duisburg/DE, P. Sela, Duisburg/DE, J. Herzler, Duisburg/DE, M. Fikri, Duisburg/DE, C. Schulz, Duisburg/DE	17:20
17:40	Is ReO₃ a mixed ionic–electronic conductor? A DFT study of defect formation and migration in a B^vO₃ perovskite-type oxide J. P. Parras, Aachen/DE	Gold Nanorods - Metal Oxide Gel Composites as SERS-Substrates B. Klemmed, Dresden/DE, A. Benad, Dresden/DE, C. Ziegler, Dresden/DE, A. Eychmüller, Dresden/DE	17:40
18:00 POSTER EVENING (even numbers)		18:00	
19:30 POSTER EVENING (odd numbers) (19:30 – 21:00)		19:30	
21:30 yPC Networking Evening		21:30	

- P 10.24 **Cationic clustering influences the phase behaviour of ionic liquids**
T. Niemann, Rostock/DE, D. Zaitsau, Rostock/DE, A. Strate, Rostock/DE, A. Villinger, Rostock/DE, R. Ludwig, Rostock/DE
- P 10.25 **Coherent enantiomer-selective population enrichment using tailored microwave fields**
M. Schnell, Hamburg/DE, C. Perez, Hamburg/DE, A. L. Steber, Hamburg/DE, S. R. Domingos, Hamburg/DE, A. Krin, Hamburg/DE, D. Schmitz, Hamburg/DE
- P 10.26 **The influence of structural flexibility on intermolecular interactions – a multi-spectroscopic approach**
M. Schnell, Hamburg/DE, M. Fatima, Hamburg/DE, C. Perez, Hamburg/DE, A. Poblitzki, Göttingen/DE, D. Bernhard, Kaiserslautern/DE, F. Dietrich, Kaiserslautern/DE, M. Suhm, Göttingen/DE, M. Gerhards, Kaiserslautern/DE
- P 10.27 **Imaging nanoscale morphology of semiconducting polymer blends with photoemission electron microscopy**
F. Niefind, Leipzig/DE, A. Neff, Leipzig/DE, K. Siefertmann, Leipzig/DE, R. Shivhare, Dresden/DE, S. Mannsfeld, Dresden/DE, B. Abel, Leipzig/DE
- P 10.28 **Deuteron quadrupole coupling constants and dynamical heterogeneities in protic ionic liquids by means of deuteron NMR spectroscopy**
P. Stange, Rostock/DE, A. E. Khudozhnikov, Novosibirsk/RU, V. Overbeck, Rostock/DE, A. Appelhagen, Rostock/DE, D. Paschek, Rostock/DE, A.G. Stepanov, Novosibirsk/RU, D. Kolokolov, Novosibirsk/RU, R. Ludwig, Rostock/DE
- P 10.29 **Disentangling the THz/FIR spectrum of small water clusters using helium nanodroplet spectroscopy**
R. Schwan, Bochum/DE, D. Mani, Bochum/DE, N. Pal, Bochum/DE, G. Schwaab, Bochum/DE, B. Redlich, Nijmegen/NL, L. v. d. Meer, Nijmegen/NL, M. Havenith, Bochum/DE
- P 10.30 **Application of X-Ray Fluorescence Holography on the Superconductor Parent β -FeTe**
B. Paulus, Marburg/DE, J. R. Stellhorn, Kumamoto/JP, S. Hosokawa, Kumamoto/JP, K. Kudo, Okayama/JP, K. Sowa, Krakow/PL, W.-C. Pilgrim, Marburg/DE
- P 10.31 **Spatially-separated conformers of a dipeptide**
N. Teschmit, Hamburg/DE, D. Horke, Hamburg/DE, J. Küpper, Hamburg/DE
- P 10.32 **Ionization Loss/Gain Stimulated Raman Spectroscopy of isolated molecules in the gas phase: diphenyl ether and bisphenyldiadamantane**
D. Maué, Kaiserslautern/DE, A. Stamm, Kaiserslautern/DE, D. Bernhard, Kaiserslautern/DE, A. A. Fokin, Giessen/DE, P. R. Schreiner, Giessen/DE, M. Gerhards, Kaiserslautern/DE
- P 10.33 **Structural investigation of $[\text{Co}_m\text{Ni}_n(\text{EtOH})_1]^+$ clusters ($1 \leq n+m \leq 4$) and implementation of a desorption source**
M. Becherer, Kaiserslautern/DE, D. Bellaire, Kaiserslautern/DE, F. Dietrich, Kaiserslautern/DE, M. Gerhards, Kaiserslautern/DE
- P 10.34 **The role of dispersion in the structure of diphenyl ether aggregates**
D. Bernhard, Kaiserslautern/DE, F. Dietrich, Kaiserslautern/DE, M. Fatima, Hamburg/DE, C. Perez, Hamburg/DE, A. Poblitzki, Göttingen/DE, C. Holzer, Karlsruhe/DE, W. Klopfer, Karlsruhe/DE, M. Suhm, Göttingen/DE, M. Schnell, Hamburg/DE, M. Gerhards, Kaiserslautern/DE

Energy Conversion and Storage

- P 11.01 **Defects in doped ceria: a computational study**
S. Grieshammer, Aachen/DE, J. Koettgen, Aachen/DE, M. Martin, Aachen/DE
- P 11.02 **Solar Energy Storage in Strained Organic Molecules: Photoelectrochemical In-Situ IR Spectroscopy of Electrochemically Controlled Norbornadiene Systems**
F. Waidhas, Erlangen/DE, O. Brummel, Erlangen/DE, M. Jevric, Göteborg/SE, K. Moth-Poulsen, Göteborg/SE, J. Bachmann, Erlangen/DE, J. Libuda, Erlangen/DE
- P 11.03 **Computational investigation of lanthanum apatites as solid state electrolytes**
T. Schultze, Aachen/DE, S. Grieshammer, Aachen/DE

POSTER PROGRAMME

- P 11.04 **Organic electroactive materials with high loading fraction for semi-solid redox flow batteries**
Z. Huang, Saarbrücken/DE, R. Hempelmann, Saarbrücken/DE, R. Chen, Saarbrücken/DE
- P 11.05 **“Water-in-ionic liquid” electrolytes boost aqueous high-voltage rechargeable battery**
Y. Zhang, Saarbrücken/DE, R. Hempelmann, Saarbrücken/DE, R. Chen, Saarbrücken/DE
- P 11.06 **Investigations on an improved state-of-charge indicator for the all-vanadium redox flow battery**
J. Geiser, Saarbrücken/DE, H. Natter, Saarbrücken/DE, R. Hempelmann, Saarbrücken/DE, B. Morgenstern, Saarbrücken/DE, K. Hegetschweiler, Saarbrücken/DE
- P 11.07 **Model studies on the dehydrogenation and decomposition of liquid organic hydrogen carriers on model catalyst surfaces by surface x-ray diffraction**
R. Schuster, Erlangen/DE, V. Vonk, Hamburg/DE, F. Waidhas, Erlangen/DE, M. Bertram, Erlangen/DE, M. A. Herráez, Hamburg/DE, H. Runge, Hamburg/DE, T. Wähler, Erlangen/DE, A. Stierle, Hamburg/DE, J. Libuda, Erlangen/DE
- P 11.08 **Metalation of 2H-Tetraphenylporphyrin on metal oxide nanoparticles: the influence of hydroxylation and hydration**
J. Schneider, Salzburg/AT, R. Restom, Salzburg/AT, T. Berger, Salzburg/AT, O. Diwald, Salzburg/AT
- P 11.09 **One-Step Mechanochemistry of Nanoglassy Oxides**
V. Sepelák, Eggenstein-Leopoldshafen/DE, E. Tóthová, Košice/SK, M. Senna, Yokohama/JP, H. Hahn, Eggenstein-Leopoldshafen/DE, P. Heitjans, Hannover/DE
- P 11.10 **Exploring Surface Phenomena of Silver Nanowire Network Electrodes and their Influence on Organic Solar Cells**
L. Sonntag, Dresden/DE, F. Eichler, Dresden/DE, N. Weiß, Dresden/DE, L. Bormann, Dresden/DE, N. Gaponik, Dresden/DE, K. Leo, Dresden/DE, A. Eychmüller, Dresden/DE
- P 11.11 **Contraction capability of light-responsive foldamers investigated by Molecular Dynamics simulations**
M. Böckmann, Münster/DE, N. Doltsinis, Münster/DE
- P 11.12 **Electronic and ionic structure of Li-ion electrode – solid electrolyte interfaces: space charge- and reaction layer formation at the LiCoO₂-LiPON interface**
R. Hausbrand, Darmstadt/DE, M. Fingerle, Darmstadt/DE, K. Albe, Darmstadt/DE, S. Siculo, Darmstadt/DE
- P 11.13 **A guideline for optimizing the microstructure of a battery electrode**
R. Usiskin, Stuttgart/DE, J. Maier, Stuttgart/DE
- P 11.14 **Neutron spectrometer NEAT at Helmholtz Zentrum Berlin – a powerful experimental tool for energy material research**
M. Russina, Berlin/DE, V. Grzimek, Berlin/DE, G. Günther, Berlin/DE, T. Kaulich, Berlin/DE, L. Drescher, Berlin/DE
- P 11.15 **Zirconium phosphate composite membrane for vanadium redox flow battery**
S. J. Yoon, Saarbrücken/DE, Y. T. Hong, Daejeon/KR, S. Kim, Saarbrücken/DE, R. Hempelmann, Saarbrücken/DE
- P 11.16 **Wet-chemical synthesis of 2D tin(II) sulfide nanosheets**
C. Bauer, Dresden/DE, S. Heckel, Dresden/DE, A. Eychmüller, Dresden/DE, V. Lesnyak, Dresden/DE
- P 11.17 **Molten-flux synthesis of La₂NiO_{4+δ}**
Z. Zhao, Hannover/DE, R. Hinterding, Hannover/DE, C. Zhang, Hannover/DE, A. Feldhoff, Hannover/DE
- P 11.18 **Self-assembly of a thermoelectric nanocomposite in a complex oxide system**
M. Bittner, Hannover/DE, N. Kanas, Trondheim/NO, F. Steinbach, Hannover/DE, D. Groneveld, Hannover/DE, R. Hinterding, Hannover/DE, P. Wemhoff, Hannover/DE, K. Wijk, Trondheim/NO, M.-A. Einarsrud, Trondheim/NO, A. Feldhoff, Hannover/DE
- P 11.19 **Oxide/Polymer-Composites for Thermoelectric Application**
M. Wolf, Hannover/DE, K. Menekse, Hannover/DE, A. Mundstock, Hannover/DE, A. Feldhoff, Hannover/DE
- P 11.20 **Entropy - A central quantity in thermoelectric energy conversion**
A. Feldhoff, Hannover/DE

ORAL SESSIONS / PRESENTATION UPLOAD

For contributed oral presentations, computers with the following software is provided: Apple macOS (10.13), Apple Keynote (7.3), Microsoft Office 2016 (16.10), Adobe Reader DC (18.11).

Upload your presentation no later than 18:00 the day prior your talk

Note that multiple sessions under the same topical name are numbered to allow for automatic upload of your presentation to the computer at the correct location and time of lecture by using the dedicated upload-link valid for your session. All upload-links are password protected with the **upload-link and password information provided by email**.

You do not need to bring you own laptop nor an USB-stick to the session since neither of them might be connected.

Friday, 11 May 2018

12:25 – 13:25

WOMEN'S NETWORKING LUNCH

Universität Hannover, Callinstr. 3A, Room 115/2504

18:00 – 21:00

POSTER SESSION & POSTER DINNER

Lichthof – University of Hannover

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

21:30

yPC – YOUNG PHYSICAL CHEMISTS NETWORKING EVENING

at the Kuriosum (Am Schneiderberg 14)

SOCIAL PROGRAMME

Thursday, 10 May 2018

- 19:30 – 22:30 **Welcome Reception at the HDI Arena**
 Panoramic Lounge, Robert-Enke-Str. 1, 30169 Hannover
 Bus transportation to the HDI Arena from the main entrance of the Leibniz University at 7:00 p.m.
Price per person: 12,00 € (incl. 19% VAT) nominal charge

Friday, 11 May 2018

- 10:00 **Tour 1: Fountain City Tour („Wenn alle Brunnlein fließen...“)**
 Meeting point: Neustädter Markt, Tischbrunnen
 End of the tour: Ständehausstraße
 Duration: 1,5 hours
Price per person: 10,00 € (language: German, English translation on advance request only)
Booking required
- 12:25 – 13:25 **Women's Networking Lunch**
 Universität Hannover, Callinstr. 3A, Room 115/2504
 KEYNOTE SPEAKER
 N. N.
Price per person: 15,00 € (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 2018. 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 relaxing 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 welcome you at the Women's Networking Lunch and ask you to register for the event jointly with your conference registration.
 The organisers, Yvonne Joseph & Melanie Schnell
- 14:00 **Tour 2: Great Gardens and Glittering Grotto („Großer Garten und glitzernde Grotte“)**
 Meeting point: Herrenhäuser Gärten, Infopavillon
 End of the tour: Herrenhäuser Gärten, Großer Garten
 Duration: 1,5 hours
Price per person: 13,50 € (language: German, English translation on advance request only)
Booking required

Saturday, 12 May 2018

- 10:00 **Tour 3: City tour with Wilhelm Busch („Eins-Zwei-Drei im Sauseschritt!“)**
 Meeting point: Ernst-August-Denkmal, Main Train Station
 End of the tour: Ballhof
 Duration: 1,5 hours
Price per person: 17,50 € (language: German, English translation on advance request only)
Booking required
- 12:25 – 13:25 **yPC-MITGLIEDERVERSAMMLUNG**
 Universität Hannover, Callinstr. 3A, Room 115/2504
- 14:00 **Tour 4: Tour through the Leibniz University („Welfenschloss und Wissenschaft“)**
 Meeting point: Main entrance University, Welfengarten 1
 End of the tour: Conti Campus, Königsworther Platz
 Duration: 2 hours
Price per person: 10,00 € (language: German, English translation on advance request only)
Booking required

REGISTRATION FEES¹⁾

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

Late registrations after 28 February 2018 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 10 May 2018 and the Poster Session and Poster Dinner on 11 May 2018 are included, no admission 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 optionally with your registration for an additional fee of 10 €), the list of participants, meals and beverages during the poster session as well as the coffee breaks.

Lunches are not included in the registration fee.

REGISTRATION

Please register online at 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 **22 April 2018**. It is not guaranteed that attendees registering past the deadline will appear in the list of participants.

PAYMENT

If fees are paid in advance, but after **23 April 2018** we kindly ask participants to show proof of payment when claiming their tickets and conference material at the conference office. Credit cards (Amex, Mastercard, VISA) and direct debit will be accepted.

CANCELLATION

Cancellations received in writing on or before **5 April 2018** will be refunded less a 25,- Euro administration fee. After that date the full amount of the invoice is owed. Requests for refund will not be accepted; however, registration may be transferred to another member of your organisation. In this case, please send a note to GDCh, Event Team.

If the conference is cancelled beforehand for unforeseeable reasons, fees paid will be refunded in full. Further recourse is excluded.

ACCOMMODATION

The Hannover Marketing und Tourismus GmbH will gladly assist in booking accommodation in all categories.

Hannover Marketing und Tourismus GmbH

Vahrenwalder Straße 7

30165 Hannover, Germany

Phone: +49 511 12345-555

Fax: +49 511 12345-556

E-mail: hotels@hannover-tourismus.de

A list of hotels with reserved room contingents can be found under the menu 'Hotel' on the conference webpage. Please note that many more budget hotels are available in addition.

The customers will be held accountable for non-occupancy of reserved rooms.

GENERAL INFORMATION

VENUE[\(Map on page 80\)](#)**Opening Session:** Audimax, Bldg. 1101, Welfenschloß**Conference office:** Room C109, Bldg. 1101**Seminar Wiley-VCH, Seminar academics:**

Leibniz Universität Hannover

Welfengarten 1

30167 Hannover/DE

Bunsen-Meetings, eDu-Forum, yPC-Karrierefórum, yPC-Mitgliederversammlung, Women's Networking Lunch:

Leibniz Universität Hannover

Institut für Physikalische Chemie

Callinstr. 3A

30167 Hannover/DE

HOW TO REACH THE VENUE[\(Map on page 80\)](#)

On the conference **website www.bunsentagung.de**, under the menu "Venue and arrival", you will find a link to the route description to the Universität Hannover (www.uni-hannover.de/de/service/wegweiser).

OPENING HOURS ON-SITE CONFERENCE OFFICE[\(Building 1101, Room C109\)](#)

Thursday, 10 May 2018 11:00 – 19:30

Friday, 11 May 2018 08:00 – 18:00

Saturday, 12 May 2018 08:00 – 16:00

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

Claudia Birkner

Gesellschaft Deutscher Chemiker e.V.

Varrentrappstr. 40-42

60486 Frankfurt am Main/DE

Phone: +49 69 7917-366

Fax: +49 69 7917-1366

E-mail: tgonline@gdch.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/DE

Phone: +49 69 7917-362

Fax: +49 69 7917-1362

E-mail: geschaefsstelle@bunsen.deInternet: 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. 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 provided.**CHILD CARE**

The Bunsentagung offers the opportunity for child care service to parents of small children during the event. Interested parents are asked to register and complete the requested information within their online registration.

INTERNET SERVICE

Free internet access will be provided via the 'eduroam' service (<https://www.eduroam.org>) or Leibniz University's 'UHEvent' service for all participants during the conference.

More and regularly updated information on the conference is available at

www.bunsentagung.de

POSTER SESSION, POSTER DINNER AND POSTER AWARDS**Friday, 11 May 2018****18:00 – 21:00**

There will be a dedicated “Poster Evening” on Friday, 11 May 2018 from 18:00 to 21:00. The session will be divided into even poster numbers (from 18:00 to 19:30) and odd poster numbers (from 19:30 to 21:00). **All authors are expected to be present at their own poster during the dedicated 1,5 hours of presentation time 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 – International Metric Standard) portrait format. Material to affix the posters will be provided on-site. 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. The presentations should be posted 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 11 presentations will be selected to receive the “Best Poster Award” of 150 € each and free admission to the Bunsentagung 2019 for the main author. The three most outstanding awardees are asked to deliver an oral presentation at the Bunsentagung 2019 in Jena, subject to the timely submission of an abstract.

The **Poster Award Ceremony** will take place during the Closing Ceremony on **Saturday 12 May 2018 at 15:55.**

Only authors present at the Closing Ceremony will be awarded.

yPC-KARRIEREFORUM (in German only)**Thursday, 10 May 2018****11:30 – 14:30**

The yPC-Forum (Karriere Seminar) is an annual symposium organised by the young Physical Chemists (yPC) of the DBG. It aims at scientists in earlier stages of their careers (between PhD and senior faculty appointment), and provides a forum for discussion on career related issues.

eDu-Forum (in German only)**Thursday, 10 May 2018****11:30 – 14:30**

Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, room 010

PROGRAMME**Akademisches Lernen und Studienerfolg in der Studieneingangsphase**

Prof. Elke Sumfleth, Didaktik der Chemie, Universität Duisburg-Essen

Physikalische Chemie ohne Mathematik (1. Semester)

Prof. Christian Mayer, Physikalische Chemie, Universität Duisburg-Essen

The Pen Is Mightier Than the Keyboard – Lückentexte in PC-Vorlesungen

Prof. Peter Gilch, Physikalische Chemie, Heinrich-Heine Universität Düsseldorf

Quizabfragen mit dem Smartphone: Beispiele aus der Kinetik

Prof. Sebastian Schlücker, Physikalische Chemie, Universität Duisburg-Essen

Inverted Classroom: Beispiel Thermodynamik (2. Semester)

Prof. Jochen Gutmann, Physikalische Chemie, Universität Duisburg-Essen

Dauerbaustelle Mathematik

Prof. Rudolf Holze, Physikalische Chemie, Techn. Universität Chemnitz

Friday, 11 May 2018**21:30 – open end**

Following the poster evening yPC invites all participants to the **Young Physical Chemists Networking Evening**. We will meet at the Kuriosum (Am Schneiderberg 14) starting at 21:30 to end the day pleasantly with some drinks, music, and the chance to connect to other young and like-minded researchers. The evening will allow developing new and maintaining old friendships.

The HCS Group GmbH generously sponsors two drinks per person (**conference registration required**).

MAP UNIVERSITY OF HANNOVER



Building 2501

Callinstr. 3
Room 133

Building 2504

Callinstr. 3A
Room 007
Room 010
Room 115

Building 1101

Welfengarten 1
Room F303
Room B302
Room B305
Room E001
Room E214
Room E415

