

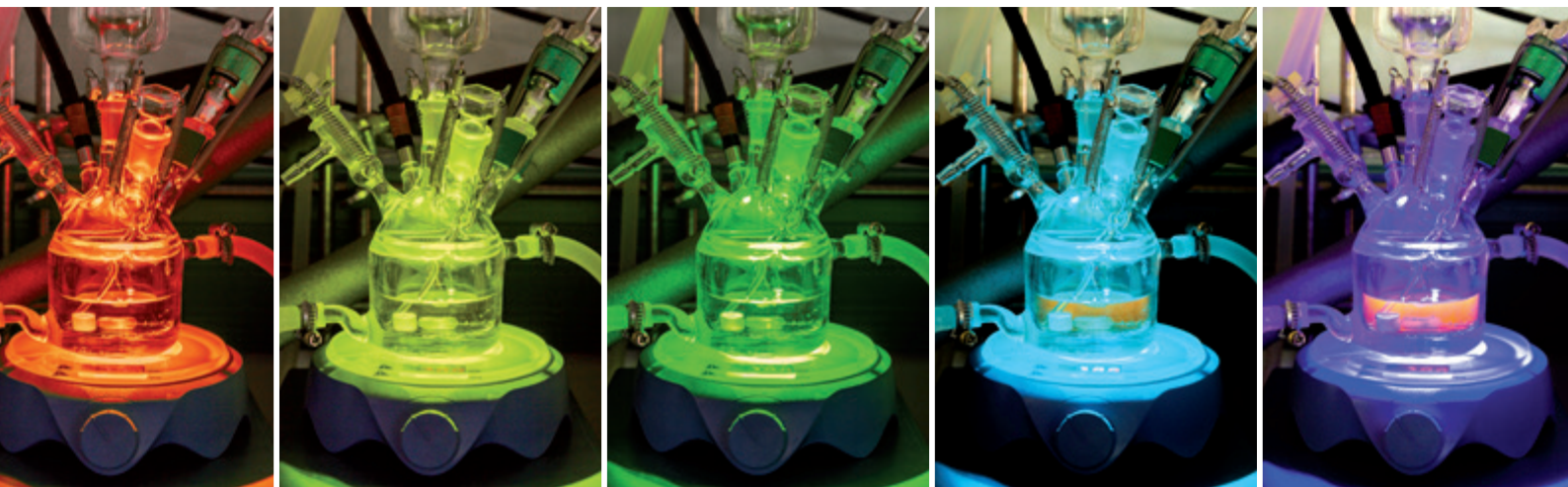


BUNSENTAGUNG 2016

115th General Assembly of the German Bunsen Society for Physical Chemistry

Featuring an industrial symposium with accompanying exhibition
and Karriereforum

5 – 7 MAY 2016 · ROSTOCK · GERMANY



PROGRAMME

Basic Mechanisms in Energy Conversion

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Universität
Rostock



Traditio et Innovatio

1218
HAFEN DER ROSTOCK
WISSENSCHAFTEN 1419

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As of 10 February 2016, subject to alterations. Submission title and authors information as given by the submitter. No proof by DBG.

MAIN TOPIC:

“Basic Mechanisms of Energy Conversion”

The sustainable generation and storage of energy is one of the most important scientific and technical challenges in the 21st century. The vanishing fossil fuel supplies need to be replaced by renewable resources. That includes avoiding the negative effects of the current energy supply system on climate, environment and health.

Among renewable energy resources, solar energy is the by far the largest exploitable resource. The sun provides more energy in one hour to the earth surface than all of the energy consumed by humans in an entire year. If solar energy is to be a major renewable energy source, it must be stored and dispatched on demand to the user. Thus capture, storage and distribution of solar-converted energy are the main scientific challenges.

Solar capture and conversion may be accomplished by photovoltaic technology, while solar electricity can be stored mechanically by pumped storage hydroelectricity or electrochemically using batteries. Wind and solar thermal energy conversion technologies are presently the by far cheapest methods of solar energy capture and conversion.

However, the most promising method for the future conversion and storage of solar energy is a design borrowed from nature. In photosynthesis, carbon dioxide and water are converted into organic molecules such as sugars and into oxygen. Although we can learn from nature, natural photosynthesis is too complex and relatively inefficient. However, part of these processes can be copied or retraced in artificial photosynthesis.

Chemical energy conversion technologies include photovoltaic applications, hydrogen storage, photocatalytic water splitting devices, development of fuel cells, hydrogen storage in small molecules, synthesis of organic molecules (methanol or methane) from fixation of atmospheric carbon dioxide. The most attractive method for energy conversion and storage is the production of cheap solar fuels.

However, harvesting solar energy and converting it to electricity or chemical fuels at low cost and using abundantly available raw materials is still a huge challenge. New technologies, methods, reactions and materials for solar energy capture and conversion are badly needed.

Thus, research and development in energy conversion and storage are becoming increasingly important. Novel materials with higher efficiencies, improved performance and superior features need to be developed.

“Energy conversion” represents an interdisciplinary field and requires combined efforts from chemistry, physics, biology, engineering and materials sciences. It is the aim of the Bunsentagung 2016 to highlight our current understanding of the basic mechanisms in energy conversion processes. This understanding at short time and small length scales is a prerequisite for designing new materials, tuning reactions and improving efficiency.

The Bunsentagung 2016 on “Basic Mechanisms in Energy Conversion” in Rostock will provide a perfect platform for fruitful research activities across many disciplines with a focus on physical and theoretical chemistry. The topic will be highlighted by an array of distinct speakers, all international experts in the field.

SCIENTIFIC ORGANISATION

Ralf Ludwig	Universität Rostock/D	Udo Kragl	Universität Rostock/D
Joachim Wagner	Universität Rostock/D	Matthias Beller	LIKAT, Rostock/D
Angelika Brückner	LIKAT, Rostock/D	Oliver Kühn	Universität Rostock/D

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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 Mrs. Carmen Weidner-Friedrich (geschaeftsstelle@bunsen.de).

LIST OF EXHIBITORS

(as of 10 February 2016)

- Belltec – Ing. Büro Glocke, Wesel/D
- Bruker Optik GmbH, Ettlingen/D
- DFG Deutsche Forschungsgemeinschaft e.V., Bonn/D
- Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin/D
- PCCP Physical Chemistry Chemical Physics, Cambridge/UK
- rhd instruments GmbH & Co. KG, Marburg/D
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FURTHER FINANCIAL SUPPORT

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- DFG Deutsche Forschungsgemeinschaft e.V., Bonn/D
- FCI Fonds der Chemischen Industrie, Frankfurt am Main/D
- SFB 652, Rostock/D
- Universität Rostock, Rostock/D

You support the conference via a direct donation to the German Bunsen Society.

Please contact Mrs Carmen Weidner-Friedrich (geschaeftsstelle@bunsen.de) for additional information.

MEETINGS OF THE GERMAN BUNSEN SOCIETY

Thursday, 5 May 2016	
10:00 – 12:00	Vorstandssitzung* (only invitational)
12:00 – 14:30	Sitzung des Ständigen Ausschusses* (only invitational)
12:00 – 15:00	Karrierefórum* „Forschung nach der Promotion“
13:00 – 15:00	Sitzung der Themenkommission*
13:00 – 15:00	Sitzung der Studienkommission*
15:00 – 16:00	Ordentliche Mitgliederversammlung* (only for DBG members)
Friday, 6 May 2016	
12:30 – 13:30	Women's Networking Lunch
Saturday, 7 May 2016	
12:30 – 13:30	Mitgliederversammlung AG Bunsen-Karrierefórum*

* in German only

Thursday, 5 May 2016		
12:00-15:00	Arno-Esch II	Karriereforum (in German only)
15:00-16:00	Arno-Esch I	Ordentliche Mitgliederversammlung (only for DBG members, in German only)
Chair	Sauer/Ludwig	
16:30-18:30	Audimax	OPENING CEREMONY
18:30-19:15		OPENING LECTURE: Grätzel
19:30-22:00		Welcome Reception

Friday, 6 May 2016								
Chair	Beller							
08:30-09:15	Audimax	PL01	PLENARY LECTURE: Xu					
	Audimax	Arno-Esch I	Arno-Esch II		Haus 1 Hörsaal 224		Haus 1 Hörsaal 323	
	Main Topic	Soft Matter and Polymers	Industrial Applications		Liquids and Solvation		Chemical Dynamics and Kinetics	
Chair	Strunk	Wagner		Plass		Urbanski		Siefermann
09:30-09:50	V01.01 Litke	V08.01	Gradzielski	V13.01	Kohnke	V02.01	Rathke	V03.01 Moshhammer
09:50-10:10	V01.02 Walenta	V08.02	Pacholski	V13.02	Egger	V02.02	Kerlé	V03.02 Wezisla
10:10-10:30	V01.03 Bredol	V08.03	Hansen	V13.03	Vargas-Barbosa	V02.03	Knorr	V03.03 Oum
10:30-10:50	V01.04 Borchert	V08.04	Plamper	V13.04	Burggraf	V02.04	Kiefer	V03.04 Hüter
10:50-11:10	COFFEE BREAK							
	Main Topic	Soft Matter and Polymers	Solids and Nano-sized Matter		Liquids and Solvation		Chemical Dynamics and Kinetics	
Chair	Ludwig	Porada		Bigall		Bande		Gerhards
11:10-11:30	FL01.01 FULL LECTURE Kornyshev	V08.05	Urbanski	V07.01	Dorfs	V02.05	Imoto	V03.05 Van der Linde
11:30-11:50		V08.06	Nack	V07.02	Kartouzian	V02.06	Knake	V03.06 Van Wilderen
11:50-12:10	V01.05 Einemann	V08.07	Herold	V07.03	Schaumberg	V02.07	Heyden	V03.07 Torres-Alacan
12:10-12:30	V01.06 Hausbrand	V08.08	Elsing	V07.04	Niedermaier	V02.08	Gleim	V03.08 Kahnt
12:30-13:30	LUNCH BREAK (12:30 – 13:30 Women's Networking Lunch, Haus 1, Raum SR021)							
Chair	Wagner							
13:30-14:15	Audimax	PL02	PLENARY LECTURE: Durrant					
	Audimax	Arno-Esch I	Arno-Esch II		Haus 1 Hörsaal 224		Haus 1 Hörsaal 323	
	Main Topic	Electrochemistry and Energy	Solids and Nano-sized Matter		Industrial Applications		Hot Topics	
Chair	Kornyshev	Hofmann		Kartouzian		Kragl		Nickel
14:30-14:50	V01.07 Chen	V12.01	Senocrate	FL07.01 FULL LECTURE Bigall	V13.05	Hartmann	V14.01	Starr
14:50-15:10	V01.08 Bickel	V12.02	Tranca		V13.06	Barsch	V14.02	Hemberger
15:10-15:30	V01.09 Neff	V12.03	dos Santos Sardinha	V07.05	Scheele	V13.07	Ondo	Pérez de Tudela
15:30-15:50	V01.10 Fischer	V12.04	Chen	V07.06	Boldt	V13.08	Joseph	V14.04 Usvyat
15:50-16:10	COFFEE BREAK							
	Main Topic	Experimental Techniques	Solids and Nano-sized Matter		Surfaces and Interfaces		Preisträgersession	
Chair	Kaiser	Lauth		Niedner-Schatteburg		Schmitt		Sauer
16:10-16:30	V01.11 Strunk	V05.01	Waldt	V07.07	Passow	V09.01	Bünemann	V15.01 Nernst-Haber-Bodenstein Preis
16:30-16:50	V01.12 Widmann	V05.02	Kottke	V07.08	Lauth	V09.02	Paier	V15.02 Paul-Bunge Preis
16:50-17:10	FL01.02 FULL LECTURE Papp	V05.03	Pramann	V07.09	Nielsen	V09.03	Yang	
17:10-17:30		V05.04	Hollmann	V07.10	Kruss	V09.04	Späth	V15.03 Ewald-Wicke Preis
17:30-17:50	V01.13 Neumann	V05.05	Zimina	V07.11	Klinke	V09.05	Kropp	V15.04 Wilhelm-Ostwald-Nachwuchspreis
	Tent							
18:00-19:30	POSTER SESSION (even numbers)							
19:30-21:00	POSTER SESSION (odd numbers)							

Saturday, 7 May 2016										
Chair	Kühn									
08:30-09:15	Audimax		PL03	PLENARY LECTURE: Lubitz						
	Audimax		Arno-Esch I		Arno-Esch II		Haus 1 Hörsaal 224		Haus 1 Hörsaal 323	
	Main Topic		Electrochemistry and Energy		Biophysical Chemistry		Surfaces and Interfaces		Molecular Structure	
Chair	Marshall		Peuckert		Kottke		Backus		Schnell	
09:30-09:50	V01.14	Lambert	V12.05	Lück	V10.01	Khadem	V09.06	Schmid	V04.01	Pitzer
09:50-10:10	V01.15	Müh	V12.06	Single	V10.02	Luong	V09.07	Atonsson	V04.02	Wiese
10:10-10:30	V01.16	Wächtler	V12.07	Wu	V10.03	Herten	V09.08	Schneider	V04.03	Reusch
10:30-10:50	V01.17	Greisch	V12.08	Berger	V10.04	Vogel	V09.09	Siebels	V04.04	Bumüller
10:50-11:10	COFFEE BREAK									
	Main Topic		Electrochemistry and Energy		Biophysical Chemistry		Surfaces and Interfaces		Molecular Structure	
Chair	Papp		Schuster		Herten		Wöll		Kühn	
11:10-11:30	V01.18	Merschjann	V12.09	Chanaewa	V10.05	Bald	FL09.01 FULL LECTURE Backus	V04.05	Poblotzki	
11:30-11:50	V01.19	Dräger	V12.10	Schedel-Niedrig	V10.06	Roder		V04.06	Bernhard	
11:50-12:10	V01.20	Feldhoff	V12.11	Taffa	V10.07	Langel	V09.10	Munoz-Santiburcio	V04.07	Schnell
12:10-12:30	V01.21	Andrei	V12.12	Pfeifer	V10.08	Müller	V09.11	Behler	V04.08	Song
12:30-13:30	LUNCH BREAK									
Chair	Kragl									
13:30-14:15	Audimax		PL04	PLENARY LECTURE: DeBeer						
	Audimax		Arno-Esch I		Arno-Esch II		Haus 1 Hörsaal 224		Haus 1 Hörsaal 323	
	Main Topic		Electrochemistry and Energy		Catalysis		Theoretical Techniques		Hot Topics	
Chair	Lochbrunner		Paschek		Beller		Paier		Dick	
14:30-14:50	V01.22	Lenzer	V12.13	Brummel	V11.01	Kubis/König	V06.01	Fabri	V14.05	Heyda
14:50-15:10	V01.23	Marschall	V12.14	Oezaslan	V11.02	Kunz	V06.02	Ivanov	V14.06	Gliemann
15:10-15:30	V01.24	Schmitt	FL12.01 FULL LECTURE Frittmann		V11.03	Wagner	V06.03	Kandratsenka	V14.07	Senske
15:30-15:50	V01.25	Kundu			V11.04	Boubnov	V06.04	Müller	V14.08	Neugeboren
16:00-16:30	Audimax		CLOSING CEREMONY / POSTER AWARD CEREMONY							

OPENING LECTURE

Thursday, 5 May 2016	
18:30 – 19:15	Mesoscopic photosystems for the solar generation of electricity and fuels M. Grätzel ¹ ; ¹ RPFL – École polytechnique fédérale de Lausanne/CH

PLENARY LECTURES

Friday, 6 May 2016	
8:30 – 9:15	Functional nanomaterials for energy conversion and storage Q. Xu, Advanced Industrial Science and Technology (AIST), Osaka/J
13:30 – 14:15	Charge carrier dynamics for photoelectrochemical water splitting J. Durrant, Imperial College London/UK

Saturday, 7 May 2016	
8:30 – 9:15	Mechanism of light-induced water oxidation and oxygen release in photosynthesis W. Lubitz, MPI für Chemische Energiekonversion, Mülheim/D
13:30 – 14:15	Making and breaking bonds: x-ray Spectroscopic studies of small molecule activation by biological catalysts S. DeBeer, MPI für Chemische Energiekonversion, Mülheim/D

FULL LECTURES

Friday, 6 May 2016	
11:10 – 11:50 FL01.01	Energy harvesting and storage with ionic liquids: the essential physics at the nanoscale A.A. Kornyshev ¹ ; ¹ Imperial College London/UK
14:30 – 15:10 FL07.01	Hydrogels and aerogels of nanocrystal building blocks <u>N. Bigall</u> ¹ ; ¹ Leibniz Universität Hannover/D
16:50 – 17:30 FL01.02	Dehydrogenation of liquid organic hydrogen carriers on Pt(111) <u>C. Papp</u> ¹ ; C. Gleichweit ¹ ; M. Amende ¹ ; S. Schernich ¹ ; W. Zhao ¹ ; M. Lorenz ¹ ; O. Höfert ¹ ; N. Brückner ¹ ; P. Wasserscheid ¹ ; J. Libuda ¹ ; H. Steinrück ¹ ; ¹ Universität Erlangen-Nürnberg, Erlangen/D

Saturday, 7 May 2016	
11:10 – 11:50 FL09.01	Two types of water at the water–surfactant interface revealed by time-resolved vibrational spectroscopy R. Livingstone ¹ ; Y. Nagata ¹ ; M. Bonn ¹ ; <u>E. Backus</u> ¹ ; ¹ Max Planck Institute for Polymer Research, Mainz/D
15:10 – 15:50 FL12.01	Investigation of co-adsorption and side processes during underpotential deposition of Cu and Ag on Au(111) by electrochemical microcalorimetry <u>S. Frittmann</u> ¹ ; V. Halka ¹ ; R. Schuster ¹ ; ¹ Karlsruhe Institute of Technology (KIT)/D

Thursday, 5 May 2016

	Room: Arno-Esch II
12:00 – 15:00	KARRIEREFORUM (in German only, see page 86)
	Room: Arno-Esch I
15:00 – 16:15	ORDENTLICHE MITGLIEDERVERSAMMLUNG DER DBG (only for DBG members, in German only)
	Room: Audimax
Chair	J. Sauer, Humboldt-Universität zu Berlin/D; R. Ludwig, Universität Rostock/D
16:30 – 18:30	OPENING CEREMONY
18:30 – 19:15	OPENING LECTURE: Mesoscopic photosystems for the solar generation of electricity and fuels M. Grätzel ¹ ; ¹ RPFL – École polytechnique fédérale de Lausanne/CH
	Room: Tent
19:30 – 22:00	WELCOME RECEPTION

Friday, 6 May 2016			Morning
	Room: Audimax		
Chair:	M. Beller, Leibniz-Institut für Katalyse e.V., Rostock/D		Chair:
08:30 PL01	PLENARY LECTURE Functional nanomaterials for energy conversion and storage Q. Xu, Advanced Industrial Science and Technology (AIST), Osaka/J		08:30 PL01
	Room: Audimax	Room: Arno-Esch I	
	Main Topic – Basic Mechanisms in Energy Conversion	Soft Matter and Polymers	
Chair:	J. Strunk, Max-Planck-Institut für chemische Energiekonversion, Mülheim/D		Chair:
09:30 V01.01	TiO₂ as a bottleneck for the photocatalytic water reduction on Cd_{0.5}Zn_{0.5}S@Pt-TiO₂ composites A. Litke ¹ ; J. Hofmann ¹ ; T. Weber ¹ ; E. Hensen ¹ ; ¹ Eindhoven University of Technology/NL	Complexes of chitosan and alkylethoxycarboxylates: pH responsive systems of versatile structure and properties M. Gradzielski ¹ ; L. Chiappisi ¹ ; M. Simon ¹ ¹ TU Berlin/D	09:30 V08.01
09:50 V01.02	Ethanol photocatalysis on rutile TiO₂(110): unraveling the mechanistic role of defects and water C. Walenta ¹ ; S. Kollmannsberger ¹ ; M. Tschurl ¹ ; U. Heiz ¹ ; ¹ TU München, Garching/D	Benefits of using hydrogel microgels in colloidal lithography C. Pacholski ¹ ; M. Weiler ² ; ¹ University of Potsdam/D; ² Max Planck Institute for Intelligent Systems, Stuttgart/D	09:50 V08.02
10:10 V01.03	Electrocatalytic activity of sulfides M. Bredol ¹ ; V. Niemann ² ; J. Goossen ¹ , ¹ Fachhochschule Münster, Steinfurt/D; ² Drexel University, Philadelphia, PA/USA	Atomistic simulations of the formation of perylene-based supramolecular complexes in aqueous solution J. Baz ¹ ; N. Hansen ¹ ; ¹ University of Stuttgart /D	10:10 V08.03
10:30 V01.04	Solar cells with a solution-processable heterojunction between CuInS₂ and ZnO nanocrystals H. Borchert ¹ ; D. Scheunemann ¹ ; S. Wilken ¹ ; R. Miranti ¹ ; C. Krause ¹ ; J. Parisi ¹ ; ¹ University of Oldenburg/D	Interface-enforced complexation between copolymer blocks A. Steinschulte ¹ ; E. Plamper ¹ ; ¹ RWTH Aachen University/D	10:30 V08.04
10:50	COFFEE BREAK		10:50
	Room: Audimax	Room: Arno-Esch I	
	Main Topic – Basic Mechanisms in Energy Conversion	Soft Matter and Polymers	
Chair:	R. Ludwig, Universität Rostock/D		Chair:
11:10 FL01.01	FULL LECTURE Energy harvesting and storage with ionic liquids: the essential physics at the nanoscale A.A. Kornyshev ¹ ; ¹ Imperial College London/UK	New insights into nematic nanocomposites by dielectric spectroscopy: conductivity, polarization and relaxation M. Bourg ¹ ; M. Urbanski ¹ ; ¹ University of Luxembourg /L	11:10 V08.05
		Hindered nematic alignment of hematite spindles in viscoelastic matrices A. Nack ¹ ; J. Seifert ¹ ; C. Passow ¹ ; J. Wagner ¹ ; ¹ University of Rostock/D	11:30 V08.06
11:50 V01.05	High temperature proton conducting fuel cell membrane additives operating under anhydrous conditions M. Einemann ¹ ; C. Harms ² ; M. Wark ¹ ; ¹ University of Oldenburg/D; ² NEXT Energy Forschungszentrum, Oldenburg/D	Viral coefficients of anisotropic, hard solids of revolution: The influence of the geometry E. Herold ¹ ; R. Hellmann ¹ ; J. Wagner ¹ ; ¹ University of Rostock/D	11:50 V08.07
12:10 V01.06	Electronic and ionic structure of Li-ion battery materials: concept and impact on interface properties R. Hausbrand ¹ ; M. Fingerle ¹ ; ¹ TU Darmstadt/D	Monodisperse, ordered polystyrene foams and their mechanical properties J. Elsing ¹ ; M. Gilchrist ² ; W. Drenckhan ³ ; C. Stubenrauch ¹ ; ¹ University of Stuttgart/D; ² University College Dublin/IRL; ³ Université Paris Sud/F	12:10 V08.08
12:30	LUNCH BREAK		12:30

Friday, 6 May 2016			Morning
	Room: Audimax		
Chair:	M. Beller, Leibniz-Institut für Katalyse e.V., Rostock/D		Chair:
08:30 PL01	PLENARY LECTURE Functional nanomaterials for energy conversion and storage Q. Xu, Advanced Industrial Science and Technology (AIST), Osaka/J		08:30 PL01
	Room: Arno-Esch II	Room: Haus 1 – Hörsaal 224	
	Industrial Applications	Liquids and Solvation	
Chair:	M. Plass, DOW Europe GmbH, Horgen/CH		Chair:
09:30 V13.01	Electrochemical potential determination H. Kohnke ¹ , ¹ Gaskatel GmbH, Kassel/D	Protic ionic liquids: mesoscopic inhomogeneities in solutions of ethyl-ammonium nitrate and n-alkyl alcohols O. Russina ¹ ; A. Triolo ² ; W. Schröer ³ ; B. Rathke ³ ; ¹ Università di Roma Sapienza, Rome/I; ² Consiglio Nazionale delle Ricerche, Rome/I; ³ Universität Bremen/D	09:30 V02.01
09:50 V13.02	La₂NiO₄ as anode material for high temperature steam electrolysis A. Egger ¹ ; N. Schrödl ¹ ; W. Sitte ¹ ; C. Gspan ² ; F. Hofer ² ; ¹ Montanuniversität Leoben/A; ² Graz University of Technology/A	A further step to the understanding of the solvation behavior of alcohols in ionic liquids. A. Appelhagen ¹ ; D. Kerlé ² ; ¹ University of Rostock/D; ² Universität Bremen/D	09:50 V02.02
10:10 V13.03	Investigating the viability of monopolar and bipolar membranes as separators in buffered water-splitting cells N. Vargas-Barbosa ¹ ; T. Mallouk ² ; ¹ Universität Marburg/D; ² The Pennsylvania State University, University Park, PA/USA	Spectroscopic evidence for clusters of like-charged ions in ionic liquids A. Knorr ¹ ; P. Stange ¹ ; R. Ludwig ¹ ; ¹ University of Rostock/D	10:10 V02.03
10:30 V13.04	Novel materials and components for Proton Exchange Membrane (PEM) water electrolysis: status and challenges F. Burggraf ¹ ; P. Lettenmeier ¹ ; A. Gago ¹ ; K. Friedrich ¹ ; ¹ DLR – German Aerospace Center, Stuttgart/D	Excess spectroscopy to study binary and ternary solutions J. Kiefer ¹ ; F. Zehentbauer ¹ ; K. Noack ² ; ¹ Universität Bremen/D; ² Universität Erlangen-Nürnberg, Erlangen/D	10:30 V02.04
10:50	COFFEE BREAK		10:50
	Room: Arno-Esch II	Room: Haus 1 – Hörsaal 224	
	Solids and Nano-sized Matter	Liquids and Solvation	
Chair:	N.-C. Bigall, Universität Hannover/D		Chair:
11:10 V07.01	Tuning the localized surface plasmon resonances in degenerately doped semiconductor nanocrystals A. Wolf ¹ ; D. Dorfs ¹ ; ¹ Universität Hannover/D	Pressure effects on solvation structure and vibrational spectroscopy of aqueous TMAO solutions S. Imoto ¹ ; H. Forbert ¹ ; D. Marx ¹ ; ¹ Ruhr-Universität Bochum/D	11:10 V02.05
11:30 V07.02	Plasmons in supported silver clusters T. Lünskens ¹ ; P. Heister ¹ ; M. Thämer ¹ ; A. Von Weber ¹ ; M. Jakob ¹ ; A. Kartouzian ¹ ; U. Heiz ¹ ; ¹ TU München, Garching/D	The impact of TMAO and urea on the H-bond dynamics under high pressure L. Knake ¹ ; H. Vondracek ¹ ; M. Havenith ¹ , ¹ Ruhr-Universität Bochum/D	11:30 V02.06
11:50 V07.03	Laser irradiation of suspensions: mechanisms of nanoparticle generation C. Schaumburg ¹ ; ¹ Humboldt-Universität zu Berlin/D	Thermodynamic properties of water solvating biomolecular surfaces M. Heyden ¹ ; ¹ Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr/D	11:50 V02.07
12:10 V07.04	Functionalization of oxide nanocrystals and composites with transition metal ions M. Niedermairer ¹ ; A. Gheisi ² ; J. Bernardi ³ ; O. Diwald ¹ ; ¹ Paris-Lodron Universität Salzburg/A; ² Universität Erlangen-Nürnberg, Erlangen/D; ³ Vienna University of Technology/A	Ultrafast dynamics of vibrational relaxation of pseudohalides in liquid-to-supercritical water. a critical test of fermi's golden rule J. Gleim ¹ ; D. Czurlok ¹ ; J. Lindner ¹ ; P. Vöhringer ¹ ; ¹ University of Bonn/D	12:10 V02.08
12:30	LUNCH BREAK		12:30

Friday, 6 May 2016		Morning
		Room: Audimax
Chair:		M. Beller, Leibniz-Institut für Katalyse e.V., Rostock/D
08:30 PL01		PLENARY LECTURE Functional nanomaterials for energy conversion and storage Q. Xu, Advanced Industrial Science and Technology (AIST), Osaka/J
		Room: Haus 1 - Hörsaal 323
		Chemical Dynamics and Kinetics
Chair:		K. Siefertmann, Leibniz-Institut für Oberflächenmodifizierung e.V., Leipzig/D
09:30 V03.01		Advancing kinetic mechanisms for low-temperature combustion through the detection of highly elusive intermediates K. Moshhammer ¹ ; A. Jasper ¹ ; N. Hansen ¹ ; ¹ Sandia National Laboratories, Livermore, CA/USA
09:50 V03.02		The primary photochemical processes of a ferrocyclobutadiene in liquid solution studied by ultrafast mid-infrared spectroscopy B. Wezislá ¹ ; J. Lindner ¹ ; P. Vöhringer ¹ ; ¹ University of Bonn/D
10:10 V03.03		A comprehensive kinetic model for the excited state dynamics of all-trans retinal O. Flender ¹ ; M. Scholz ¹ ; J. Hölzer ¹ ; T. Lenzer ¹ ; K. Oum ¹ ; ¹ University of Siegen/D
10:30 V03.04		Vibronic coherence in the first excited $\pi\pi^*$ state of penta-fluorobenzene by coupling to the $\pi\sigma^*$ state Q. Hüter ¹ ; M. Sala ¹ ; H. Neumann ¹ ; S. Zhang ¹ ; H. Studzinski ¹ ; D. Egorova ¹ ; F. Temps ¹ ; ¹ Kiel University/D
10:50		COFFEE BREAK
		Room: Haus 1 - Hörsaal 323
		Chemical Dynamics and Kinetics
Chair:		M. Gerhards, TU Kaiserslautern/D
11:10 V03.05		Photochemistry of organic compounds adsorbed on salt clusters C. van der Linde ¹ ; N. Bersenkowitsch ¹ ; M. Beyer ¹ ; ¹ University of Innsbruck/A
11:30 V03.06		Picosecond photorelease mechanism of coumarin-cages to trigger ultrafast bio/chemical processes L. van Wilderen ¹ ; C. Neumann ¹ ; D. Kern-Michler ¹ ; N. Seibert ¹ ; A. Rodrigues Correia ¹ ; M. Reinfelds ¹ ; A. Heckel ¹ ; J. Bredenbeck ¹ ; ¹ University of Frankfurt/D
11:50 V03.07		o-Benzynes: An elusive intermediate investigated by time-resolved FTIR spectroscopy J. Torres-Alacan ¹ ; ¹ University of Bonn/D
12:10 V03.08		Radiation chemical modification of graphene oxide A. Kahnt ¹ ; S. Eigler ² ; R. Flyunt ³ ; W. Knolle ³ ; S. Naumov ³ ; B. Abel ³ ; ¹ Universität Erlangen-Nürnberg, Erlangen/D; ² Chalmers University of Technology, Gothenburg/S; ³ Leibniz Institute of Surface Modification (IOM), Leipzig/D
12:30		LUNCH BREAK

Friday, 6 May 2016		Afternoon
		Room: Audimax
Chair:		J. Wagner, Universität Rostock/D
13:30 PL02		PLENARY LECTURE Charge carrier dynamics for photoelectrochemical water splitting J. Durrant, Imperial College London/UK
		Room: Arno-Esch I
		Electrochemistry and Energy
Chair:		J.P. Hofmann, TU Eindhoven/NL
14:30 V01.07	Structural insights into charged Li₂-xMO₂F by synchrotron X-ray PDF and XANES R. Chen ¹ ; R. Hempelmann ² ; E. Maawad ³ ; M. Yavuz ⁴ ; M. Knapp ⁴ ; S. Zander ⁵ ; ¹ KIST Europe, Saarbrücken/D; ² Saarland University, Saarbrücken/D; ³ Helmholtz-Zentrum Geesthacht (HZG), Hamburg/D; ⁴ Karlsruhe Institute of Technology (KIT)/D; ⁵ Helmholtz-Zentrum Berlin (HZB)/D	Unraveling the nature of ionic conductivity in hybrid organic-inorganic halide perovskites A. Senocrate ¹ ; T. Yang ¹ ; G. Gregori ¹ ; N. Pellet ² ; M. Graetzel ² ; J. Maier ¹ ; ¹ Max Planck Institute for Solid State Research, Stuttgart/D; ² Ecole Polytechnique Fédérale de Lausanne/CH
14:50 V01.08	Insights into the mechanism of the pyridine catalyzed electro-chemical CO₂ reduction K. Bickel ¹ ; A. Crespo-Yapur ¹ ; M. Daimer ¹ ; S. Filser ¹ ; Q. Li ¹ ; K. Schönleber ¹ ; K. Krischer ¹ ; ¹ TU München, Garching/D	Codoped 2D conjugated metal-organic surface for efficient electrochemical hydrogen production: from molecules to solid catalysts D. Tranca ¹ ; R. Dong ¹ ; I. Tranca ² ; N. Chandrasekhar ¹ ; H. Liang ¹ ; J. Zhang ¹ ; S. Liu ¹ ; G. Seifert ¹ ; Z. Zheng ¹ ; X. Feng ¹ ; ¹ TU Dresden/D; ² Eindhoven University of Technology/NL
15:10 V01.09	Imaging ultrafast photo-induced dynamics in semiconducting polymer films with time-resolved photoemission electron microscopy A. Neff ¹ ; K. Siefertmann ¹ ; ¹ Leibniz Institute of Surface Modification, Leipzig/D	Removal of the SiO₂ native layer from silicon electrodes – scanning electrochemical microscopy and X-ray photoelectron spectroscopy E. dos Santos Sardinha ¹ ; H. Büler ¹ ; G. Wittstock ¹ ; ¹ University of Oldenburg/D
15:30 V01.10	Mechanistic Understanding of photocatalytic water reduction with iron carbonyl phosphines by means of in situ spectroscopy and time dependent - DFT calculations. S. Fischer ¹ ; A. Lennox ² ; O. Bokareva ¹ ; A. Rösel ¹ ; N. Rockstroh ² ; M. Bauer ³ ; O. Kühn ¹ ; M. Beller ² ; R. Ludwig ¹ ; ¹ University of Rostock/D; ² Leibniz-Institut für Katalyse e.V., Rostock/D; ³ Paderborn University /D	Mass storage at heterojunctions C. Chen ¹ ; R. Usiskin ¹ ; L. Fu ¹ ; J. Maier ¹ ; ¹ Max Planck Institute for Solid State Research, Stuttgart/D
15:50		COFFEE BREAK
		Main Topic - Basic Mechanisms in Energy Conversion
Chair:		B. Kaiser TU Darmstadt/D
16:10 V01.11	Identification and exclusion of intermediates of photocatalytic CO₂ reduction on TiO₂ under conditions of highest purity A. Pougin ¹ ; M. Dilla ² ; J. Strunk ² ; ¹ Ruhr-Universität Bochum/D; ² Max-Planck-Institute for Chemical Energy Conversion, Mülheim a.d. Ruhr/D	Gas phase studies of luminescent lanthanoid complexes by trapped ion laser induced fluorescence (TLIF) E. Waldt ¹ ; J. Greisch ¹ ; B. Schäfer ¹ ; M. Ruben ¹ ; M. Kappes ² ; D. Schooss ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Karlsruhe Institute of Technology (KIT)/D
16:30 V01.12	Methanol formation via CO₂ hydrogenation on Au/ZnO catalysts – influence of CO and its role in the reaction mechanism D. Widmann ¹ ; ¹ Ulm University/D	Indirect isotope effects need to be taken into account for the assignment of vibrational spectra of complex molecules T. Domratcheva ¹ ; E. Hartmann ¹ ; I. Schlichting ¹ ; C. Sommer ² ; M. Dietz ² ; T. Kottke ² ; ¹ Max Planck Institute for Medical Research, Heidelberg/D; ² Bielefeld University/D
16:50 FL01.02	FULL LECTURE Dehydrogenation of liquid organic hydrogen carriers on Pt(111) C. Papp ¹ ; C. Gleichweit ¹ ; M. Amende ¹ ; S. Schernich ¹ ; W. Zhao ¹ ; M. Lorenz ¹ ; O. Höfert ¹ ; N. Brückner ¹ ; P. Wasserscheid ¹ ; J. Libuda ¹ ; H. Steinrück ¹ ; ¹ Universität Erlangen-Nürnberg, Erlangen/D	The role of HR-MC-ICP mass spectrometry in the redefinition of the SI unit kilogram A. Pramann ¹ ; O. Rienitz ¹ ; ¹ Physikalisch-Technische Bundesanstalt (PTB), Braunschweig/D
		New spectroscopic in situ tools for monitoring electrocatalysts during water oxidation (WO) D. Hollmann ¹ ; K. Grabow ¹ ; J. Rabeah ¹ ; M. Polyakov ¹ ; A. Sukrus ¹ ; U. Bentrup ¹ ; S. Klink ² ; W. Schuhmann ² ; A. Brückner ¹ ; ¹ Leibniz-Institut für Katalyse e.V., Rostock/D; ² Ruhr-Universität Bochum/D
17:30 V01.13	Mechanism of the aqueous-phase reforming of methanol – understanding the role of the base E. Alberico ¹ ; A. Lennox ² ; L. Neumann ² ; H. Jiao ² ; W. Baumann ² ; H. Drexler ² ; M. Nielson ² ; H. Junge ² ; M. Beller ² ; ¹ Istituto di Chimica Biomolecolare, Sassari/I; ² Leibniz-Institut für Katalyse e.V., Rostock/D	The CAT-ACT beamline at ANKA: a new high energy X-ray spectroscopy facility for CAtalysis and ACTinide research A. Zimina ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
		Room: Tent
18:00		POSTER SESSION (even numbers)
19:30		POSTER SESSION (odd numbers) (19:30 – 21:00)

Friday, 6 May 2016		Afternoon
	Room: Audimax	
Chair:	J. Wagner, Universität Rostock/D	Chair:
13:30 PL02	PLENARY LECTURE Charge carrier dynamics for photoelectrochemical water splitting J. Durrant, Imperial College London/UK	13:30 PL02
	Room: Arno-Esch II	Room: Haus 1 - Hörsaal 224
	Solids and Nano-sized Matter	Industrial Applications
Chair:	A. Kartouzian, TU München/D	Chair:
14:30 FL07.01	FULL LECTURE Hydrogels and aerogels of nanocrystal building blocks N. Bigall ¹ ; ¹ Leibniz Universität Hannover/D	14:30 V13.05
	FTIR spectroelectrochemistry – details of equipment and applications W. Hartmann ¹ ; M. Kessler ¹ ; ¹ Bruker Optik GmbH, Ettlingen/D	
	Application of in situ infrared spectroscopy to the production of a flavouring substance E. Barsch ¹ ; A. Petri ² ; P. Müller ² ; R. Ludwig ¹ ; ¹ University of Rostock/D; ² Miltitz Aromatics GmbH, Bitterfeld-Wolfen/D	14:50 V13.06
15:10 V07.05	Conductive PbS mesocrystals A. André ¹ ; M. Samadi Khoshkhoo ¹ ; M. Weber ¹ ; M. Scheele ¹ ; ¹ University of Tübingen/D	15:10 V13.07
15:30 V07.06	Environmental effects on the stability and photo-chemistry of semiconductor nanocrystals K. Boldt ¹ ; N. Kirkwood ² ; S. Murphy ² ; J. Baldauf ² ; P. Mulvaney ² ; ¹ University of Konstanz/D; ² University of Melbourne & Bio21 Institute, Melbourne/AUS	15:30 V13.08
15:50	COFFEE BREAK	15:50
	Solids and Nano-sized Matter	Surfaces and Interfaces
Chair:	G. Niedner-Schatteburg, TU Kaiserslautern/D	Chair:
16:10 V07.07	Orientational distribution functions of suspended spindle-shaped hematite particles in external magnetic fields C. Passow ¹ ; A. Nack ¹ ; J. Wagner ¹ ; ¹ University of Rostock/D	16:10 V09.01
16:30 V07.08	Ultrafast dynamics of electron-hole pairs in 2D InSe nanosheets J. Lauth ¹ ; F. Spoor ¹ ; A. Kulkarni ¹ ; A. Houtepen ¹ ; J. Schins ¹ ; S. Kíngé ² ; L. Siebbeles ¹ ; ¹ Delft University of Technology/NL; ² Toyota Motor Europe, Delft/NL	16:30 V09.02
16:50 V07.09	Small-diameter semiconductor block nanowires synthesized by Solution-Liquid-Solid (SLS) technique and cation exchange A. Nielsen ¹ ; W. Buhro ² ; T. Kipp ¹ ; A. Mews ¹ ; ¹ Uinversität Hamburg/D; ² Washington University in St. Louis, MO/USA	16:50 V09.03
17:10 V07.10	Impact of redox-active molecules on fluorescence and exciton dynamics in semiconducting carbon nanotubes S. Kruss ¹ ; ¹ Universität Göttingen/D	17:10 V09.04
17:30 V07.11	Electrical transport through colloidal PbS sheets C. Klinke ¹ ; ¹ University of Hamburg/D	17:30 V09.05
	Room: Tent	
18:00	POSTER SESSION (even numbers)	18:00
19:30	POSTER SESSION (odd numbers) (19:30 – 21:00)	19:30

Friday, 6 May 2016		Afternoon
	Room: Audimax	
Chair:	J. Wagner, Universität Rostock/D	Chair:
13:30 PL02	PLENARY LECTURE Charge carrier dynamics for photoelectrochemical water splitting J. Durrant, Imperial College London/UK	13:30 PL02
	Room: Haus 1 – Hörsaal 323	
	Hot Topics	
Chair:	U. Nickel HCS GmbH, Frankfurt/D	Chair:
14:30 V14.01	Soft and hard X-ray ambient pressure X-ray photoelectron spectroscopic characterization of the BiVO₄/potassium phosphate interface for water splitting applications D. Starr ¹ ; F. Abdi ¹ ; M. Favaro ² ; M. Kanis ¹ ; H. Bluhm ² ; E. Crumlin ² ; R. van de Krol ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D; ² Lawrence Berkeley National Laboratory, Berkeley, CA/USA	14:30 V14.01
14:50 V14.02	Threshold photoelectron spectroscopy to trace chemistry in combustion, pyrolysis and catalysis P. Hemberger ¹ ; ¹ Paul Scherrer Institut (PSI), Villigen PSI/D	14:50 V14.02
15:10 V14.03	Dissociation of microsolvated acids R. Pérez de Tudela ¹ ; D. Marx ¹ ; ¹ Ruhr-Universität Bochum/D	15:10 V14.03
15:30 V14.04	Hierarchical quantum chemical treatment as a path to sub-kJ/mol accuracy in solid-state applications D. Usvyat ¹ ; ¹ Universität Regensburg/D	15:30 V14.04
15:50	COFFEE BREAK	15:50
	Award Session	
Chair:	J. Sauer, Humboldt-Universität zu Berlin/D	Chair:
16:10 V15.01	Nernst-Haber-Bodenstein Preis	16:10 V15.01
16:30 V15.02	Paul-Bunge Preis	16:30 V15.02
17:10 V15.03	Ewald-Wicke Preis	17:10 V15.03
17:30 V15.04	Wilhelm-Ostwald-Nachwuchspreis	17:30 V15.04
	Room: Tent	
18:00	POSTER SESSION (even numbers)	18:00
19:30	POSTER SESSION (odd numbers) (19:30 – 21:00)	19:30

Saturday, 7 May 2016			Morning	
	Room: Audimax			
Chair:	O. Kühn, Universität Rostock/D		Chair:	
08:30 PL03	PLENARY LECTURE Mechanism of light-induced water oxidation and oxygen release in photosynthesis W. Lubitz, MPI für Chemische Energiekonversion, Mülheim/D		08:30 PL03	
	Room: Audimax	Room: Arno-Esch I		
	Main Topic – Basic Mechanisms in Energy Conversion	Electrochemistry and Energy		
Chair:	R. Marschall, Universität Gießen/D		Chair:	
09:30 V01.14	On the spin chemistry of donor-acceptor triads containing transition metal photosensitisers <u>C. Lambert</u> ¹ ; ¹ University of Würzburg/D	Modeling of adsorption processes at nanostructured cathodes in lithium-sulfur batteries <u>J. Lück</u> ¹ ; A. Latz ¹ ; ¹ German Aerospace Center (DLR), Ulm/D	09:30 V12.05	
09:50 V01.15	Linking structure and optical spectra of photosynthetic pigment-protein complexes <u>F. Müh</u> ¹ ; ¹ University of Linz/A	Modelling SEI growth: a novel description for porous layers <u>F. Single</u> ¹ ; B. Horstmann ¹ ; A. Latz ¹ ; ¹ German Aerospace Center (DLR), Ulm/D	09:50 V12.06	
10:10 V01.16	Multimetallic terpyridine complexes with highly conjugated ligands for spatially directed energy transport <u>M. Wächter</u> ¹ ; J. Kübel ¹ ; K. Barthelmes ² ; A. Winter ² ; A. Schmiedel ³ ; C. Lambert ⁴ ; U. Schubert ² ; B. Dietzek ¹ ; ¹ Leibniz Institute of Photonic Technology, Jena/D; ² University of Jena/D; ³ Universität Würzburg, Jena/D; ⁴ University of Würzburg/D	Graphene-based nanocomposites with hierarchical structures as high-performance electrodes for lithium (sodium) storage <u>C. Wu</u> ¹ ; ¹ Max Planck Institute for Solid State Research, Stuttgart/D	10:10 V12.07	
10:30 V01.17	Gas-phase photoluminescence characterization of mass-selected lanthanoid complexes: energy transfer mechanisms <u>J. Greisch</u> ¹ ; M. Harding ¹ ; J. Chmela ² ; B. Schäfer ¹ ; M. Ruben ¹ ; W. Kloppe ² ; D. Schooss ¹ ; M. Kappes ² ; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Karlsruhe Institute of Technology (KIT)/D	Defects in porous networks of WO₃ particle aggregates A. Márquez ¹ ; M. Rodríguez-Pérez ² ; J. Anta ³ ; G. Rodríguez-Gattorno ² ; G. Bourret ¹ ; G. Oskam ² ; <u>T. Berger</u> ¹ ; ¹ University of Salzburg/A; ² CINVESTAV-IPN, Mérida, Yucatán/MEX; ³ Universidad Pablo de Olavide, Seville/E	10:30 V12.08	
10:50	COFFEE BREAK		10:50	
	Room: Audimax	Room: Arno-Esch I		
	Main Topic – Basic Mechanisms in Energy Conversion	Electrochemistry and Energy		
Chair:	C. Papp, Universität Erlangen-Nürnberg, Erlangen/D		Chair:	
11:10 V01.18	Graphitic carbon nitrides as graphene complements: new insights and challenges <u>C. Merschjann</u> ¹ ; ¹ Freie Universität Berlin/D	Charge redistribution and extraction in photocatalytically synthesized Au–ZnO nanoppyramids <u>A. Chanaewa</u> ¹ ; ¹ VU University Amsterdam/NL	11:10 V12.09	
11:30 V01.19	Titanium and Iron substituted LiCoTi_xMn_{1-x}O₄/ LiCo_{1-y}Fe_yMnO₄: energy storage via high-voltage spinels <u>C. Dräger</u> ¹ ; S. Indris ² ; H. Ehrenberg ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Karlsruhe Institute of Technology (KIT)/D	Novel, efficient and stable composite photoelectrodes based on device-grade silicon and chalcopyrite for visible-light driven hydrogen and oxygen evolution <u>T. Schedel-Niedrig</u> ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D	11:30 V12.10	
11:50 V01.20	Energy conversion in thermo-ionic-electronic materials and systems <u>A. Feldhoff</u> ¹ ; ¹ Leibniz Universität Hannover/D	Dye molecules induced porosity in electrodeposited zinc ferrite films for enhanced photoelectrochemical response <u>D. Taffa</u> ¹ ; M. Wark ¹ ; ¹ University of Oldenburg/D	11:50 V12.11	
12:10 V01.21	Environmentally friendly composites for flexible thermoelectrics: concepts and applications <u>V. Andrei</u> ¹ ; K. Bethke ¹ ; K. Rademann ¹ ; ¹ Humboldt-Universität zu Berlin/D	The electronic structure of iridium oxides active in water splitting <u>V. Pfeifer</u> ¹ ; T. Jones ¹ ; J. Velasco-Vélez ² ; R. Arrigo ² ; M. Hävecker ² ; A. Knop-Gericke ¹ ; R. Schlögl ¹ ; ¹ Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D; ² Max-Planck-Institut für Chemische Energiekonversion, Mülheim a. d. Ruhr/D	12:10 V12.12	
12:30	LUNCH BREAK		12:30	

Saturday, 7 May 2016			Morning	
	Room: Audimax			
Chair:	O. Kühn, Universität Rostock/D		Chair:	
08:30 PL03	PLENARY LECTURE Mechanism of light-induced water oxidation and oxygen release in photosynthesis W. Lubitz, MPI für Chemische Energiekonversion, Mülheim/D		08:30 PL03	
	Room: Arno-Esch II	Room: Haus 1 - Hörsaal 224		
	Biophysical Chemistry	Surfaces and Interfaces		
Chair:	T. Kottke, Universität Bielefeld/D		Chair:	
09:30 V10.01	Distinguishing different diffusion behaviors by novel analysis of FCS autocorrelation curves <u>S. Jebreil Khadem</u> ¹ ; C. Hille ² ; H. Löhmannsröben ² ; I. Sokolov ¹ ; ¹ Humboldt-Universität zu Berlin/D; ² University of Potsdam/D	Using the molecular structure of a tetrapyrrole ligand to tune the oxidation state of metal ions: Co(III)- and Ni(III)-corroles on Ag(111) <u>M. Schmid</u> ¹ ; M. Zugermeier ¹ ; M. Chen ¹ ; F. Niefind ¹ ; J. Herritsch ¹ ; R. Tonner ¹ ; J. Gottfried ¹ ; ¹ Universität Marburg/D	09:30 V09.06	
09:50 V10.02	Combined temperature, pressure, and cosolvent effects on enzyme activity <u>T. Luong</u> ¹ ; R. Winter ¹ ; ¹ TU Dortmund/D	Surface composition of free mixed nanoscale aerosols <u>E. Antonsson</u> ¹ ; B. Langer ¹ ; C. Raschpichler ¹ ; D. Marchenko ¹ ; E. Rühl ¹ ; ¹ Freie Universität Berlin/D	09:50 V09.07	
10:10 V10.03	Counting and beyond – what information is in the photon statistics? <u>D. Herten</u> ¹ ; K. Großmayer ¹ ; S. Bierbaum ¹ ; ¹ Heidelberg University/D	Porphyrin adsorption studies on metal oxide nanoparticles <u>J. Schneider</u> ¹ ; J. Bernardi ² ; T. Berger ¹ ; O. Diwald ¹ ; ¹ Paris-Lodron University Salzburg/A; ² Vienna University of Technology/A	10:10 V09.08	
10:30 V10.04	Determination of the ionization threshold of oligonucleotides and sequence-specific VUV-induced DNA strand breaks using the DNA origami technique <u>S. Vogel</u> ¹ ; J. Rackwitz ¹ ; A. Milosavljevic ² ; A. Giuliani ³ ; I. Bald ¹ ; ¹ University of Potsdam/D; ² University of Belgrade, Pregrevica/SRB; ³ Synchrotron SOLEIL, Paris/F	Coupling of quantum well emission to surface plasmon modes in rolled-up microtubes <u>J. Siebels</u> ¹ ; H. Vu ² ; A. Mews ² ; T. Kipp ² ; ¹ Universität Hamburg, Krummhörn/D; ² Universität Hamburg/D	10:30 V09.09	
10:50	COFFEE BREAK		10:50	
	Room: Arno-Esch II	Room: Haus 1 - Hörsaal 224		
	Biophysical Chemistry	Surfaces and Interfaces		
Chair:	D.-P. Herten, Universität Heidelberg/D		Chair:	
11:10 V10.05	DNA origami nanostructures as a platform for optical spectroscopy <u>I. Bald</u> ¹ ; L. Olejko ¹ ; J. Prinz ¹ ; C. Heck ¹ ; ¹ University of Potsdam/D	FULL LECTURE Two types of water at the water–surfactant interface revealed by time-resolved vibrational spectroscopy R. Livingstone ¹ ; Y. Nagata ¹ ; M. Bonn ¹ ; <u>E. Backus</u> ¹ ; ¹ Max Planck Institute for Polymer Research, Mainz/D	11:10 FL09.01	
11:30 V10.06	Local tissue manipulation using a force- and pressure-controlled AFM micropipette in a frontloading mode <u>P. Roder</u> ¹ ; C. Hille ¹ ; ¹ University of Potsdam/D			
11:50 V10.07	Networking of biopolymers – molecular dynamics on collagen and glycosaminoglycans. <u>W. Langel</u> ¹ ; E. Peter ¹ ; N. Geist ¹ ; ¹ University of Greifswald/D	Prebiotic chemistry in nanoconfined water <u>D. Muñoz-Santiburio</u> ¹ ; D. Marx ¹ ; ¹ Ruhr-Universität Bochum/D	11:50 V09.10	
12:10 V10.08	Unravelling an underrated noncovalent interaction in proteins through single-conformation IR spectroscopy of model peptides in the molecular beam <u>C. Müller</u> ¹ ; P. Walsh ² ; T. Zwiér ² ; ¹ Ruhr-Universität Bochum/D; ² Purdue University, West Lafayette, IN/USA	Molecular dynamics simulations of solid-liquid interfaces employing high-dimensional neural network potentials S. Kondati Natarajan ¹ ; V. Quaranta ¹ ; M. Hellström ¹ ; <u>J. Behler</u> ¹ ; ¹ Ruhr-Universität Bochum/D	12:10 V09.11	
12:30	LUNCH BREAK		12:30	

Saturday, 7 May 2016		Morning
		Room: Audimax
Chair:		O. Kühn, Universität Rostock/D
08:30 PL01		PLENARY LECTURE Mechanism of light-induced water oxidation and oxygen release in photosynthesis W. Lubitz, MPI für Chemische Energiekonversion, Mülheim/D
		Room: Haus 1 – Hörsaal 323
		Molecular Structure
Chair:		M. Schnell, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg/D
09:30 V04.01		Direct determination of absolute stereochemical configuration by coulomb explosion imaging M. Pitzer ¹ ; M. Kunitski ² ; T. Jahnke ² ; H. Schmidt-Böcking ² ; R. Dörner ² ; M. Schöffler ² ; S. Marquardt ³ ; S. Marquardt ³ ; R. Berger ³ ; ¹ University of Kassel, /D; ² University of Frankfurt/D; ³ Universität Marburg/D
09:50 V04.02		Molecular-frame photoelectron imaging of controlled complex molecules J. Wiese ¹ ; S. Trippel ¹ ; J. Küpper ¹ ; ¹ Center for Free-Electron Laser Science, Hamburg/D
10:10 V04.03		Distinction of structural isomers by means of chirped femtosecond laser ionization N. Reusch ¹ ; V. Krein ¹ ; N. Wollscheid ¹ ; K. Weitzel ¹ ; ¹ Universität Marburg/D
10:30 V04.04		Influence of hydrogen addition on the structures of Ruthenium cluster anions D. Bumüller ¹ ; E. Waldt ¹ ; A. Hehn ¹ ; R. Ahlrichs ¹ ; M. Kappes ¹ ; D. Schooss ¹ ; ¹ Karlsruhe Institute of Technology (KIT)/D
10:50		COFFEE BREAK
		Room: Haus 1 – Hörsaal 323
		Molecular Structure
Chair:		O. Kühn, Universität Rostock/D
11:10 V04.05		Reversed OH shifts in oxygen and π hydrogen bonded dimers of methanol with furan derivatives A. Poblotzki ¹ ; M. Suhm ¹ ; ¹ Universität Göttingen/D
11:30 V04.05		The bonus of dispersion – the diphenyl ether-methanol complex investigated using a multi-spectroscopic and theoretical approach D. Bernhard ¹ ; A. Poblotzki ² ; C. Medcraft ³ ; C. Holzer ⁴ ; A. Stamm ¹ ; F. Dietrich ¹ ; J. Altnöder ² ; M. Heger ² ; S. Zinn ³ ; M. Suhm ² ; M. Schnell ³ ; W. Kloppe ⁴ ; M. Gerhards ¹ ; ¹ TU Kaiserslautern/D; ² Universität Göttingen/D; ³ Max Planck Institute for the Structure and Dynamics of Matter, Hamburg/D; ⁴ Karlsruhe Institute of Technology (KIT)/D
11:50 V04.05		Characterization of microsolvated polycyclic-aromatic hydrocarbons and crown ethers from broadband rotational spectroscopy A. Steber ¹ ; C. Perez ¹ ; J. Lopez ² ; A. Rijs ³ ; M. Schnell ¹ ; ¹ Max Planck Institute for the Structure and Dynamics of Matter, Hamburg/D; ² Universidad de Valladolid, Valladolid/E; ³ Radboud Universiteit, Nijmegen/NL
12:10 V04.05		Vibrational spectroscopy of titanium oxide anions: structure-reactivity relationship X. Song ¹ ; ¹ Fritz-Haber-Institut der MPG, Berlin/D
12:30		LUNCH BREAK

Saturday, 7 May 2016		Afternoon
		Room: Audimax
Chair:		U. Kragl, Universität Rostock/D
13:30 PL04		PLENARY LECTURE Making and breaking bonds: X-ray Spectroscopic studies of small molecule activation by biological catalysts S. DeBeer, MPI für Chemische Energiekonversion, Mülheim/D
		Room: Audimax
		Room: Arno-Esch I
		Basic Mechanisms in Energy Conversion
		Electrochemistry and Energy
Chair:		S. Lochbrunner, Universität Rostock/D
14:30 V01.22	Charge carrier dynamics of methylammonium lead iodide: From PbI₂-rich to low-dimensional broadly emitting perovskites J. Klein ¹ ; O. Flender ¹ ; M. Scholz ¹ ; K. Oum ¹ ; T. Lenzer ¹ ; ¹ University of Siegen/D	Low platinum group metal fuel cell catalysts: from surface science to <i>in-situ</i> spectroelectrochemistry O. Brummel ¹ ; F. Waidhas ¹ ; F. Faisal ¹ ; R. Fiala ² ; M. Vorokhta ² ; I. Khalakhan ² ; G. Kovács ³ ; S. Kozlov ³ ; K. Neyman ³ ; V. Matolin ² ; J. Libuda ¹ ; ¹ Universität Erlangen-Nürnberg, Erlangen/D; ² Charles University in Prague/CZ; ³ Universitat de Barcelona/E
14:50 V01.23	Improved charge carrier separation in barium tantalate composites investigated by laser flash photolysis J. Schneider ¹ ; K. Niktin ² ; D. Bahnemann ² ; R. Marschall ³ ; ¹ Leibniz Universität Hannover/D; ² Saint-Petersburg State University/RU and Leibniz Universität Hannover/D; ³ Giessen University/D	Electrochemical degradation mechanisms of shape-controlled platinum nanoparticles M. Oezaslan ¹ ; I. Safo ¹ ; J. Haverkamp ¹ ; ¹ University of Oldenburg/D
15:10 V01.24	About the evaluation and simulation of solar energy M. Schmitt ¹ ; F. Heib ¹ ; ¹ Saarland University, Saarbrücken/D	FULL LECTURE Investigation of co-adsorption and side processes during underpotential deposition of Cu and Ag on Au(111) by electrochemical microcalorimetry S. Frittmann ¹ ; V. Halka ¹ ; R. Schuster ¹ ; ¹ Karlsruhe Institute of Technology (KIT)/D
15:30 V01.25	Ab-initio prediction of pure and mixture gas adsorption of small gas molecules in CPO-27-Mg A. Kundu ¹ ; J. Sauer ¹ ; K. Sillar ² ; ¹ Humboldt Universität zu Berlin/D; ² University of Tartu/EST	
		Room: Audimax
16:00		CLOSING CEREMONY – POSTER AWARD CEREMONY

Saturday, 7 May 2016		Afternoon
	Room: Audimax	
Chair:	U. Kragl, Universität Rostock/D	Chair:
13:30 PL04	PLENARY LECTURE Making and breaking bonds: X-ray Spectroscopic studies of small molecule activation by biological catalysts S. DeBeer, MPI für Chemische Energiekonversion, Mülheim/D	13:30 PL04
	Room: Arno-Esch II	Room: Haus 1 - Hörsaal 224
	Catalysis	Theoretical Techniques
Chair:	M. Beller, Leibniz-Institut für Katalyse e.V., Rostock/D	J. Paier, Humboldt-Universität zu Berlin/D
14:30 V11.01	In situ FTIR measurements and applied chemometrics for studying kinetic and mechanistic aspects of alkene hydroformylation C. Kubis ¹ ; M. König ¹ ; M. Sawall ² ; D. Selent ¹ ; R. Ludwig ² ; K. Neymeyr ² ; D. Hess ³ ; R. Franke ⁴ ; A. Börner ¹ ; ¹ Leibniz-Institut für Katalyse, Rostock/D; ² University of Rostock/D; ³ Evonik Performance Materials GmbH, Marl/D; ⁴ Evonik Performance Materials GmbH, Rostock/D	The quantum dynamics of tunneling and electroweak parity violation in trisulfane (HSSSH) C. Fabri ¹ ; L. Horny ¹ ; M. Quack ¹ ; ¹ ETH Zürich/CH
14:50 V11.02	Ligands on nanoparticles – combining the benefits of homogeneous and heterogeneous catalysis? S. Kunz ¹ ; ¹ University of Bremen/D	Caldeira-leggett model description of condensed phase vibrational spectroscopy S. Ivanov ¹ ; F. Gottwald ¹ ; K. Oliver ¹ ; ¹ University of Rostock/D
15:10 V11.03	Synthesis and characterization of Ni-O_x and Ni-N_x catalysts for electrochemical water splitting S. Wagner ¹ ; J. Ziegler ¹ ; B. Kaiser ¹ ; W. Jaegermann ¹ ; ¹ TU Darmstadt/D	Independent-electron surface hopping study of the nonadiabatic energy transfer at scattering NO molecule from Au(111) surface A. Kandratsenka ¹ ; B. Krüger ¹ ; T. Schäfer ¹ ; a. Wodtke ¹ ; ¹ Universität Göttingen/D
15:30 V11.04	Uncovering deactivation mechanisms of Pd-Pt catalysts for methane oxidation by X-ray absorption and infrared spectroscopy A. Boubnov ¹ ; A. Gremminger ¹ ; M. Casapu ¹ ; O. Deutschmann ¹ ; J. Grunwaldt ¹ ; ¹ Karlsruhe Institute of Technology (KIT)/D	High energy resolution X-ray absorption spectroscopy and TD-DFT calculations on copper systems P. Müller ¹ ; M. Bauer ¹ ; ¹ Paderborn University/D
	Room: Audimax	
16:00	CLOSING CEREMONY – POSTER AWARD CEREMONY	16:00

Saturday, 7 May 2016		Afternoon
	Room: Audimax	
Chair:	U. Kragl, Universität Rostock/D	Chair:
13:30 PL04	PLENARY LECTURE Making and breaking bonds: X-ray Spectroscopic studies of small molecule activation by biological catalysts S. DeBeer, MPI für Chemische Energiekonversion, Mülheim/D	13:30 PL04
	Room: Haus 1 – Hörsaal 323	
	Hot Topics	
Chair:	B. Dick, Universität Regensburg/D	Chair:
14:30 V14.05	Thermodynamic description of salt-specific effects in thermoresponsive polymers and copolymers J. Heyda ¹ ; J. Dzubiella ² ; R. Chudoba ² ; B. Schulz ² ; ¹ University of Chemistry and Technology, Prague/CZ; ² Helmholtz-Zentrum Berlin (HZB)/D	14:30 V06.01
14:50 V14.06	SURMOFs – highly porous materials with huge potential in sensor device application H. Dr. Gliemann ¹ ; C. Wölfe ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Karlsruhe Institute of Technology (KIT)/D	14:50 V06.02
15:10 V14.07	A thermodynamic study of different cosolute effects on the stability of RNase A M. Senske ¹ ; D. Constantinescu ¹ ; H. Weingärtner ¹ ; C. Herrmann ¹ ; S. Ebbinghaus ¹ ; M. Havenith ¹ ; ¹ Ruhr-Universität Bochum/D	15:10 V06.03
15:30 V14.08	Ion imaging of reaction dynamics at surfaces: Eley-Rideal vs Langmuir-Hinshelwood J. Neugebahren ¹ ; D. Harding ¹ ; H. Hahn ¹ ; D. Auerbach ¹ ; T. Kitsopoulos ¹ ; A. Wodtke ² ; ¹ Universität Göttingen/D	15:30 V06.04
	Room: Audimax	
16:00	CLOSING CEREMONY – POSTER AWARD CEREMONY	16:00

Main Topic – Basic Mechanisms in Energy Conversion	
P01-01	Rate and routes of electron transfer in an enzymatic fuel cell A. Petrenko ¹ ; M. Stein ¹ ; ¹ Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
P01-02	Viscosity dependence of hydrogen atom self-exchange: a CW-ESR line broadening study on N-hydroxyphtalimid/ phtalimide-N-oxyl J. Bächle ¹ ; ¹ Graz University of Technology/A
P01-03	Electron transfer dynamics of indoline and triarylamine sensitizers on mesoporous ZnO, TiO₂ and Al₂O₃ surfaces O. Flender ¹ ; J. Klein ¹ ; M. Scholz ¹ ; K. Oum ¹ ; T. Lenzer ¹ ; ¹ University of Siegen/D
P01-04	<i>In situ</i> spectroelectrochemical study on the oxidation of a 4H-imidazole-ruthenium dye on TiO₂ electrodes Y. Zhang ¹ ; S. Kupfer ² ; L. Zedler ¹ ; J. Schindler ¹ ; T. Bocklitz ² ; J. Guthmuller ³ ; S. Rau ⁴ ; B. Dietzek ¹ ; ¹ Leibniz Institute of Photonic Technology Jena and University of Jena/D; ² University of Jena/D; ³ Gdansk University of Technology/PL; ⁴ University of Ulm/D
P01-05	<i>In-situ</i> investigations on the norbornadiene/quadricyclane energy storage system on various metal surfaces by UPS and high-resolution-XPS U. Bauer ¹ ; ¹ Universität Erlangen-Nürnberg, Erlangen/D
P01-06	Oxidation state control of MnO_x thin films for water oxidation catalysis by pH value adjustment during the deposition process M. Shaker ¹ ; M. Khan ¹ ; M. Tesch ¹ ; J. Xiao ¹ ; L. Spiccia ² ; E. Aziz ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D; ² Monash University, Clayton/AUS
P01-07	Photocurrent of BiVO₄ is limited by surface recombination, not surface catalysis C. Zachäus ¹ ; F. Abdi ¹ ; R. van de Krol ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D
P01-08	Unraveling elementary steps of an Ir-based photocatalytic cycle for water splitting O. Bokareva ¹ ; G. Grell ¹ ; S. Bokarev ¹ ; O. Kühn ¹ ; ¹ Universität Rostock/D
P01-09	Concentration effects on the entropy of electrochemical lithium deposition: implications for Li⁺ solvation S. Matthias ¹ ; J. Xu ¹ ; J. Lindner ¹ ; P. Novák ² ; R. Schuster ¹ , ; ¹ Karlsruhe Institute of Technology (KIT)/D; ² Paul Scherrer Institut (PSI), Villigen PSI/CH
P01-10	Temperature programmed high-resolution X-ray photoelectron spectroscopy of formic acid on Ni(111) and Pt(111) P. Bachmann ¹ ; ¹ Universität Erlangen-Nürnberg, Erlangen /D
P01-11	Towards understanding the mechanism of water splitting on TiO₂ S. Hosseinpour ¹ ; ¹ Max Planck Institute for Polymer Research, Mainz/D
P01-12	Recombination spectroscopy of organic photovoltaic devices M. Eckardt ¹ ; R. Wieczorek ¹ ; F. Laquai ² ; W. Harnett ³ ; ¹ Universität Mainz, Mainz/D; ² King Abdullah University of Science and Technology (KAUST), Thuwal/SAR; ³ Universität Osnabrück/D
P01-13	Physicochemical energy conversion to phase separation, conformational isomerisation or thermal energy change. G. Ahn-Ercan ¹ ; ¹ ComputeChem und Universität Regensburg, Saal an der Donau/D
P01-14	Photon-stimulated processes on gallium nitride semiconductors S. Kollmannsberger ¹ ; C. Walenta ¹ ; M. Tschurl ¹ ; U. Heiz ¹ ; S. Weiszer ¹ ; A. Winnerl ¹ ; R. Pereira ¹ ; M. Stutzmann ¹ ; ¹ TU München, Garching/D
P01-15	Plasma enhanced CVD preparation of CoO_xOH₂ and CoMO_xOH₂ (M=Ni,Fe) as catalysts for the oxygen evolution reaction N. Weidler ¹ ; ¹ TU Darmstadt/D
P01-16	Structural investigations on a copper containing OLED complex by application of time-resolved step-scan FTIR spectroscopy and quantum chemical calculations M. Zimmer ¹ ; F. Dietrich ¹ ; F. Böppler ¹ ; M. Wallesch ² ; D. Volz ³ ; S. Bräse ² ; R. Diller ¹ ; M. Gerhards ¹ ; ¹ TU Kaiserslautern /D; ² Karlsruhe Institute of Technology (KIT)/D; ³ Cynora gmbH, Bruchsal/D
P01-17	Photoelectrochemical properties of CdS and CdSe/CdS nanorods J. Miethe ¹ ; ¹ Leibniz Universität Hannover/D

P01-18	Electrochemical interphase formation at a buried sample/electrode interface M. Schäfer ¹ ; V. Wesp ¹ ; J. Martin ¹ ; K. Weitzel ¹ ; ¹ Universität Marburg /D
P01-19	Electrodeposited nickel nanoparticles as catalysts for hydrogen evolution reaction S. Tao ¹ ; F. Yang ¹ ; B. Kaiser ¹ ; W. Jaegermann ¹ ; ¹ TU Darmstadt/D
P01-20	Ultrafast photo-induced electron transfer in self-assembled donor-acceptor coordination cages J. Ahrens ¹ ; G. Clever ² ; M. Frank ² ; D. Schwarzer ¹ ; ¹ Max-Planck-Institute for Biophysical Chemistry, Göttingen/D; ² Universität Göttingen/D
P01-21	Inelasticity in Hydrogen atom scattering from surfaces: a probe for energy conversion Y. Dorenkamp ¹ ; H. Jiang ¹ ; A. Wodtke ¹ ; O. Bünermann ¹ ; ¹ Universität Göttingen/D
P01-22	Monitoring reactive layers inside redox hydrogels by Raman microspectroscopy C. Klinkhammer ¹ ; S. Stapf ¹ ; N. Plumeré ¹ ; M. Havenith ¹ ; ¹ Ruhr University Bochum/D
P01-23	Investigation of Pt- and Pt/Ni-nanoparticles as catalysts for the hydrogen evolution reaction in electrochemical cells J. Ziegler ¹ ; F. Tabary ¹ ; L. Wittern ² ; H. Weller ² ; W. Jaegermann ¹ ; B. Kaiser ¹ ; ¹ TU Darmstadt/D; ² Universität Hamburg/D
P01-24	Imaging photo-induced processes in organic-inorganic perovskites L. Martinez Uriarte ¹ ; A. Neff ¹ ; F. Meier ² ; C. Deibel ² ; K. Siefertmann ¹ ; ¹ Leibniz Institute of Surface Modification, Leipzig/D; ² TU Dresden/D
P01-25	Understanding the effect of Ir(III/IV) aquo complexes on the photoelectrochemistry of IrO_x•nH₂O–based water-splitting cells N. Vargas-Barbosa ¹ ; T. Mallouk ² ; L. Jensen ² ; ¹ Universität Marburg/D; ² The Pennsylvania State University, University Park, PA/USA
P01-26	Group III-phosphide semiconductors for water splitting: surface preparation and water adsorption experiments A. Hajduk ¹ ; M. Lebedev ² ; B. Kaiser ¹ ; W. Jaegermann ¹ ; ¹ TU Darmstadt, Darmstadt/D; ² Ioffe Institute, St. Petersburg/RUS
P01-27	Atomistic modeling of light induced surface relief gratings M. Böckmann ¹ ; N. Doltsinis ¹ ; ¹ Universität Münster, Münster/D
P01-28	(Self)assembling amphiphilic dyes and tuning of photonic properties via morphology control M. Presselt ¹ ; S. Das ¹ ; F. Herrmann ¹ ; M. Hupfer ¹ ; B. Dietzek ¹ ; ¹ University Jena/D
P01-29	Ultrafast excited state dynamics of iridium(III) photosensitizers S. Tschierlei ¹ ; A. Neubauer ² ; N. Rockstroh ³ ; M. Karnahl ¹ ; H. Junge ³ ; M. Beller ³ ; S. Lochbrunner ² ; ¹ University of Stuttgart/D; ² University of Rostock/D; ³ Leibniz-Institut für Katalyse, Rostock/D
P01-30	Real-time observation of Ir photosensitizer reductive quenching during light-activated molecular catalysis A. Britz ¹ ; T. Assefa ¹ ; A. Galler ¹ ; W. Gawelda ¹ ; E. Bajnóczi ² ; Z. Nemeth ² ; G. Vankó ² ; N. Rockstroh ³ ; H. Junge ³ ; M. Beller ³ ; G. Doumy ⁴ ; A. March ⁴ ; S. Southworth ⁴ ; S. Bokarev ⁵ ; S. Lochbrunner ⁵ ; O. Kühn ⁵ ; C. Bressler ¹ ; ¹ European XFEL, Hamburg/D; ² Wigner Research Centre for Physics, Budapest/H; ³ Leibniz-Institut für Katalyse, Rostock/D; ⁴ Argonne National Laboratory, Argonne, IL/USA; ⁵ Universität Rostock/D
P01-31	Light-driven electron transfer in a photocatalytic model system based on a Copper photosensitizer A. Friedrich ¹ ; S. Luo ² ; H. Junge ³ ; M. Beller ³ ; S. Lochbrunner ¹ ; ¹ Universität Rostock/D; ² State Key Laboratory Breeding Base of Green Chemistry-Synthesis Technology, Zhejiang University of Technology, Hangzhou/CN; ³ Leibniz-Institut für Katalyse, Rostock/D
P01-32	In-operando atomic force microscopy for energy materials characterization F. Hausen ¹ ; ¹ Forschungszentrum Jülich GmbH/D
P01-33	SURMOFs/CNCs as tuneable “designer solids” for light harnessing and energy applications E. Redel ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
P01-34	New reaction pathway on rutile B. Jasper ¹ ; M. Osmic ² ; S. Schmiedekind ¹ ; ¹ University of Oldenburg/D; ² University of Oldenburg, Wilhelmshaven/D
P01-35	Enhanced stability of thin film silicon tandem solar cells based photocathodes with amorphous TiO₂ layers coated with nanoparticle catalysts for solar hydrogen evolution E. Yang ¹ ; L. Movsesyan ² ; F. Urbain ³ ; J. Becker ³ ; M. Toimil-Molaes ² ; B. Kaiser ¹ ; W. Jaegermann ¹ ; ¹ TU Darmstadt/D; ² GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt/D; ³ Forschungszentrum Jülich GmbH/D

Liquids and Solvation	
P02-01	Ionic dynamics in alkylammonium nitrates are decoupled from viscosity <u>S. Roy</u> ¹ ; M. Bonn ¹ ; J. Hunger ¹ ; ¹ Max Planck Institute for Polymer Research, Mainz/D
P02-02	A molecular dynamics simulation study of direct cation-cation interactions in cholinium based ionic liquids <u>J. Neumann</u> ¹ ; R. Ludwig ¹ ; D. Paschek ¹ ; ¹ Universität Rostock/D
P02-03	Structure and dynamics in mixtures of protic ionic liquids: a molecular dynamics simulation study <u>B. Golub</u> ¹ ; D. Paschek ¹ ; R. Ludwig ¹ ; ¹ Universität Rostock/D
P02-04	Temperature dependence of computed osmotic second virial coefficients of apolar solutes in aqueous solutions <u>E. Reiter</u> ¹ ; ¹ Universität Rostock/D
P02-05	Under pressure – amorphous ice – a MD simulation study <u>M. Jehser</u> ¹ ; M. Seidl ² ; T. Loerting ² ; G. Zifferer ¹ ; ¹ University of Vienna/A; ² University of Innsbruck/A
P02-06	Investigation of the formation of pharmaceutical nanoparticles within RESS by means of molecular dynamics simulation <u>S. Braun</u> ¹ ; T. Kraska ¹ ; ¹ University of Cologne/D
P02-07	Nuclear quantum effects on charge transfer in the hydrogen bond of gas phase dimers and liquid water <u>C. Schran</u> ¹ ; O. Marsalek ² ; T. Markland ² ; ¹ Ruhr-Universität Bochum/D; ² Stanford University, CA/USA
P02-08	Terpene-based mixtures: molecular insights into the solid-liquid equilibria <u>M. Alves da Rocha</u> ¹ ; F. Zehentbauer ¹ ; B. Rathke ¹ ; J. Kiefer ¹ ; ¹ Universität Bremen/D
P02-09	Imidazolium based ionic liquids: impact of cation symmetry on the liquid – liquid phase behavior of solutions with n-alkyl alcohols <u>M. Alves da Rocha</u> ¹ ; D. Kerlé ¹ ; W. Schröer ¹ ; B. Rathke ¹ ; ¹ Universität Bremen/D
P02-10	Role of hydrogen bond donors in the formation of liquid mixtures <u>M. Alves da Rocha</u> ¹ ; F. Zehentbauer ¹ ; L. Zubeir ² ; B. Rathke ¹ ; M. Kroon ² ; J. Kiefer ¹ ; ¹ Universität Bremen/D; ² Eindhoven University of Technology/NL
P02-11	THz absorption spectroscopy of an insect lipoprotein ice nucleator reveals a long-range influence on the hydrogen bond dynamics <u>A. Bäumer</u> ¹ ; J. Duman ² ; M. Havenith ¹ ; ¹ Ruhr-Universität Bochum/D; ² University of Notre Dame, IN/USA
P02-12	Probing the acidity and solvent polarity of ionic liquids by determining the spectroscopic features of the proton sensitive dye N-methyl-6-oxyquinolone <u>S. Schmode</u> ¹ ; A. Petrosyan ¹ ; R. Ludwig ¹ ; ¹ Universität Rostock/D
P02-13	Towards understanding glycan-assisted protein stabilization <u>S. Schäfer</u> ¹ ; H. Wirtz ¹ ; C. Hoberg ¹ ; J. Savolainen ¹ ; M. Havenith ¹ ; ¹ Ruhr-Universität Bochum/D
P02-14	How does spatial confinement influence proton-transfer dynamics? E. Eisbein ¹ ; G. Seifert ¹ ; T. Lorenz ¹ ; <u>J. Joswig</u> ¹ ; ¹ TU Dresden/D
P02-15	Investigation of ubiquitin using time-resolved kinetic thz absorption spectroscopy with temperature jumps <u>H. Wirtz</u> ¹ ; S. Schäfer ¹ ; C. Hoberg ¹ ; J. Savolainen ¹ ; M. Havenith ¹ ; ¹ Ruhr-Universität Bochum/D
P02-16	Photoionization of sodium doped crystalline water clusters T. Zeuch ¹ ; <u>C. Dierking</u> ¹ ; ¹ Universität Göttingen/D
P02-17	Determination of the electronic structure of aqueous urea and its derivatives: a combined soft x-ray – DFT approach M. Tesch ¹ ; R. Golnak ¹ ; <u>F. Ehrhard</u> ¹ ; R. Chuboda ¹ ; J. Dzubiella ¹ ; D. Schön ¹ ; J. Xiao ¹ ; A. Bande ¹ ; E. Aziz ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D
P02-18	Solubility convergence and criticality in ionic liquids <u>M. Namayandeh Jorabchi</u> ¹ ; D. Kerlé ² ; R. Ludwig ¹ ; D. Paschek ¹ ; ¹ University of Rostock/D; ² University of Bremen/D
P02-19	Deuteron quadrupole coupling constants and reorientational correlation times in protic ionic liquids by means of NMR relaxation time experiments, DFT-calculations and molecular dynamics simulations <u>M. Strauch</u> ¹ ; V. Overbeck ¹ ; A. Bonsa ¹ ; B. Golub ¹ ; D. Michalik ¹ ; D. Paschek ¹ ; R. Ludwig ¹ ; ¹ University of Rostock/D
P02-20	Critical radius of supercooled water droplets: on the transition towards dendritic freezing <u>S. Bauerecker</u> ¹ ; <u>T. Buttersack</u> ¹ ; ¹ TU Braunschweig/D

Chemical Dynamics and Kinetics	
P02-21	Quantifying dispersion forces in protic ionic liquids by means of low frequency spectroscopy <u>P. Stange</u> ¹ ; K. Fumino ¹ ; A. Knorr ¹ ; R. Ludwig ¹ ; ¹ Universität Rostock/D
P02-22	Molecular topology and local dynamics govern the viscosity of imidazolium-based ionic liquids Y. Zhang ¹ ; L. Xue ² ; F. Khabaz ² ; R. Doerfler ¹ ; <u>E. Quitevis</u> ² ; R. Khare ² ; E. Maginn ¹ ; ¹ University of Notre Dame, IN/USA; ² Texas Tech University, Lubbock, TX/USA
P02-23	Shear thinning of critical fluctuations in solutions of ionic liquids <u>W. Schröer</u> ¹ ; ¹ Universität Bremen/D
P03-01	Reactants induced dynamic responses of heterogeneous catalysts monitored by adsorption microcalorimetry <u>S. Wrabetz</u> ¹ ; T. Lunkenbein ¹ ; V. Pfeifer ¹ ; T. Jones ¹ ; J. Noack ¹ ; K. Mette ¹ ; A. Trunschke ¹ ; A. Knop-Gericke ¹ ; R. Schlögl ¹ ; ¹ Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D
P03-02	Theoretical investigation of the thermolysis of urea <u>D. Gratzfeld</u> ¹ ; M. Olzmann ¹ ; ¹ Karlsruher Institut für Technologie (KIT)/D
P03-03	Fuel-structure dependence of soot precursor formation processes in non-premixed laminar opposed-flow diffusion flames <u>L. Ruwe</u> ¹ ; K. Kohse-Höinghaus ¹ ; ¹ Universität Bielefeld/D
P03-04	Thermal decomposition of propene – a shock-tube and modeling study <u>L. Golka</u> ¹ ; I. Weber ¹ ; M. Olzmann ¹ ; ¹ Karlsruher Institut für Technologie (KIT)/D
P03-05	Experimental and detailed kinetic modeling study of ammonia combustion <u>S. Vallabhuni</u> ¹ ; L. Arnas ¹ ; F. Ravi ¹ ; ¹ Physikalisch-Technische Bundesanstalt (PTB), Braunschweig/D
P03-06	Observation of b₂ symmetry vibrational levels of the SO₂ $\tilde{C}^1B_2$ state <u>B. Park</u> ¹ ; J. Jiang ² ; C. Saladrigas ² ; R. Field ² ; ¹ Universität Göttingen/D; ² Massachusetts Institute of Technology, Cambridge, MA/USA
P03-07	Ultrafast species-selective photochemistry in mixtures <u>D. Kern-Michler</u> ¹ ; C. Neumann ¹ ; N. Seibert ¹ ; L. van Wilderen ¹ ; M. Reinfelds ¹ ; J. von Cosel ¹ ; A. Heckel ¹ ; I. Burghardt ¹ ; J. Bredenbeck ¹ ; ¹ Universität Frankfurt/D
P03-08	Stretching-libration dynamics in the methanol dimer <u>M. Heger</u> ¹ ; M. Suhm ¹ ; J. Andersen ² ; R. Wugt Larsen ² ; ¹ Universität Göttingen, /D; ² Technical University of Denmark, Copenhagen/DK
P03-09	Ultrafast ionization and fragmentation dynamics of chloromethylsilanes <u>E. Antonsson</u> ¹ ; I. Halfpap ¹ ; C. von Randow ¹ ; C. Raschpichler ¹ ; E. Rühl ¹ ; ¹ Freie Universität Berlin/D
P03-10	Femtosecond time-resolved dynamics of trans-methyl cinnamate by photoelectron imaging <u>J. Kus</u> ¹ ; O. Hüter ¹ ; F. Temps ¹ ; ¹ Universität zu Kiel/D
P03-11	Geometric optimization of ICD electron emitter properties in quantum dots <u>E. Weber</u> ¹ ; E. Fasshauer ² ; A. Lode ³ ; A. Bande ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D; ² University of Tromsø/N; ³ University of Basel/CH
P03-12	Influence of the biofuel isomers diethyl ether and n-butanol on pollutant formation in premixed n-butane flames <u>J. Pieper</u> ¹ ; M. Zeng ¹ ; L. Tran ¹ ; I. Graf ¹ ; K. Kohse-Höinghaus ¹ ; ¹ Bielefeld University/D
P03-13	Direct detection of CN radicals in the NCN reaction system behind shock waves <u>S. Hesse</u> ¹ ; N. Faßheber ¹ ; G. Friedrichs ¹ ; ¹ Universität zu Kiel/D
P03-14	VIPER 2D-IR spectroscopy on coumarins: selectivity experiments and simulations <u>C. Neumann</u> ¹ ; L. van Wilderen ¹ ; D. Kern-Michler ¹ ; N. Seibert ¹ ; J. von Cosel ¹ ; R. Binder ¹ ; M. Reinfelds ¹ ; I. Burghardt ¹ ; A. Heckel ¹ ; J. Bredenbeck ¹ ; ¹ Universität Frankfurt/D
P03-15	Strong field control of the interatomic coulombic decay process in quantum dots <u>A. Haller</u> ¹ ; Y. Chiang ² ; E. Aziz ¹ ; A. Bande ¹ ; ¹ Helmholtz-Zentrum Berlin (HZB)/D; ² The Chinese University of Hong Kong, Shatin, N.T./HK
P03-16	2-Butanone as an advanced biofuel - assessment of potential combustion emissions <u>C. Hemken</u> ¹ ; ¹ Bielefeld University/D

- P03-17 **Measuring the kinetics of chemical reactions on metal surfaces in a molecular beam surface scattering experiment**
[H. Hahn](#)¹; J. Neugebohren¹; D. Harding¹; D. Auerbach¹; T. Kitsopoulos¹; A. Wodtke¹; ¹ Universität Göttingen/D
- P03-18 **Experimental analysis of the passivation kinetics in aluminium**
[M. Weimerskirch](#)¹; T. Nagy¹; U. Pacher¹; W. Kautek¹; ¹ University of Vienna/A
- P03-19 **High resolution analysis and quantum dynamics of fluoroform**
[I. Bolotova](#)¹; O. Ulenikov²; E. Bekhtereva²; S. Albert¹; H. Hollenstein¹; M. Quack¹; ¹ ETH Zürich/CH; ² Tomsk Polytechnic University, Tomsk/RUS
- P03-20 **Alignment- and orientation-dynamics of ground-state selected OCS**
[S. Trippel](#)¹; ¹ Deutsches Elektronen Synchrotron DESY, Hamburg/D
- P03-21 **Investigation of the methane number as measure for knock propensity of natural gas mixtures containing higher hydrocarbons**
[L. Arnas](#)¹; S. Vallabhuni¹; R. Fernandes¹; ¹ Physikalisch-Technische Bundesanstalt (PTB), Braunschweig/D
- P03-22 **Towards understanding ultrafast dynamics in complex systems like nanodiamonds or switchable polymer nanoparticles**
[D. Hintzen](#)¹; ¹ Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig/D
- P03-23 **The photodissociation of dimethylnitrosamine revisited – a 3d-REMPI and VMI study**
[M. Schneider](#)¹; U. Kensy¹; B. Dick¹; ¹ Universität Regensburg/D

Molecular Structure

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[S. Peukert](#)¹; M. Gil¹; M. Kijak¹; J. Ostapko¹; J. Sepiol¹; J. Waluk¹; M. Broquier²; A. Zehnacker-Rentien²; ¹ Polish Academy of Sciences, Warszawa/PL; ² CNRS, Institut des Sciences Moléculaires d’Orsay (ISMO), Centre Laser Université Paris-Sud (CLUPS), University Paris-Sud, Orsay/F
- P04-02 **Excited state intramolecular proton transfer of 2,5-bis(5-ethyl-2-benzoxazolyl)-hydroquinone and its OH/OD-isotopomers studied in Supersonic jets**
[S. Peukert](#)¹; M. Gil¹; M. Kijak¹; J. Sepiol¹; ¹ Polish Academy of Sciences, Warszawa/PL
- P04-03 **Nitrogen nanocoating effects on the conformational preferences of ethanol and its dimer detected by supersonic jet spectroscopy**
[S. Oswald](#)¹; M. Suhm¹; ¹ Universität Göttingen/D
- P04-04 **Control over the hydrogen bond docking site in anisole by ring alkylation and halogenation**
[H. Gottschalk](#)¹; M. Suhm¹; ¹ Universität Göttingen/D
- P04-05 **Three views on three xylene molecules: far-infrared spectroscopy, computational chemistry, and spectral modeling**
[A. Bande](#)¹; I. Bravic¹; C. Minnich²; L. Puskar¹; E. Ritter³; U. Schade¹; E. Aziz¹; ¹ Helmholtz-Zentrum Berlin (HZB)/D; ² S-PACT GmbH, Aachen/D; ³ Humboldt-Universität zu Berlin/D
- P04-06 **Structural investigations on a linear depsipeptide by combined IR/UV spectroscopy in a molecular beam**
[A. Stamm](#)¹; D. Bernhard¹; M. Gerhards¹; ¹ TU Kaiserslautern/D
- P04-07 **Novel, heteroleptic copper(II)-4*H*-imidazolate complexes: synthesis and characterization of their structural, spectral and redox properties**
[M. Schulz](#)¹; F. Dröge¹; Y. Zhang²; C. Reichardt²; F. Herrmann-Westendorf¹; J. Schindler²; H. Görls¹; M. Presselt¹; B. Dietzek¹; ¹ Universität Jena, Jena/D; ² Leibniz-Institut für Photonische Technologien e.V., Jena/D
- P04-08 **Characterization of the cis- / trans-isomerization of peptide bond models in the gas phase**
[T. Forsting](#)¹; K. Otto¹; M. Suhm¹; ¹ Universität Göttingen/D
- P04-09 **Study of molecular interactions using broadband rotational spectroscopy**
[M. Fatima](#)¹; ¹ Max Planck Institute for Structure and Dynamics of Matter, Hamburg/D
- P04-10 **Millimeter-wavelength rotational spectroscopy for applications in astrochemistry**
[B. Arenas](#)¹; ¹ Max Planck Institute for the Structure and Dynamics of Matter, Hamburg/D
- P04-11 **Catching hydrides spectroscopically with hard X-rays**
[L. Burkhardt](#)¹; ¹ Universität Paderborn/D

- P04-12 **The role of dispersion forces for the stability of methane and carbon dioxide gas hydrates**
[W. Polet](#)¹; R. Ludwig¹; ¹ Universität Rostock/D
- P04-13 **Gas phase vibrational spectroscopy of microhydrated sulfate dianions revisited**
[H. Knorke](#)¹; ¹ Universität Leipzig/D
- P04-14 **High-resolution spectrum of the asymmetric C-H stretch of CH₂Br₂: CRDS measurements and simulations**
[I. Sadiek](#)¹; G. Friedrichs¹; ¹ Universität zu Kiel/D
- P04-15 **High resolution GHz and THz (FTIR) spectroscopy and theory of parity violation and tunneling for dithiine as a candidate for measuring the parity violating energy difference between enantiomers of chiral molecules**
[I. Bolotova](#)¹; [A. Sieghard](#)¹; Z. Chen¹; C. Fábri¹; L. Horny¹; M. Quack¹; G. Seyfang¹; D. Zindel¹; ¹ ETH Zürich/CH
- P04-16 **Single-conformation IR spectroscopy of jet-cooled sulfanilamide and its homo- and heteromolecular 1:1 clusters**
[T. Uhlemann](#)¹; S. Seidel¹; C. Müller¹; ¹ Ruhr-Universität Bochum/D
- P04-17 **Spectral signatures of polarons and dynamics of charge separation in conjugated co-polymers**
[C. Wiebeler](#)¹; S. Schumacher¹; ¹ Universität Paderborn/D
- P04-18 **Single-conformation spectroscopy, DFT, NBO, and charge density studies of the neuraminidase inhibitor analogue BANA 113**
[S. Seidel](#)¹; T. Uhlemann¹; M. Seitz²; C. Müller¹; ¹ Ruhr-University Bochum/D; ² University of Tübingen/D
- P04-19 **Influence of thermal fluctuations for the 2D-IR structure determination in the liquid phase**
[K. Fehre](#)¹; D. Kern-Michler¹; S. Combe²; P. Schreiner²; B. Kirchner³; J. Bredenbeck¹; ¹ Universität Frankfurt/D; ² Universität Gießen/D; ³ Universität Bonn/D
- P04-20 **Photochemical dissociation of HOBr. a nonadiabatic dynamics study**
[B. Allehyani](#)¹; R. Hilal¹; S. Aziz¹; ¹ King Abdulaziz University, Jeddah/SAR

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[R. Schepper](#)¹; M. Bauer¹; ¹ Universität Paderborn/D
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[K. Schlag](#)¹; D. Nattland¹; A. Timm¹; R. Schuster¹
Karlsruhe Institute of Technology (KIT)/D
- P05-03 **Contactless microwave conductivity of oxide supported metal samples**
[E. Wolf](#)¹; T. Risse²; R. Schlögl¹; S. Cap¹; ¹ Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D; ² Freie Universität Berlin/D
- P05-04 **Sensing of light induced magnetization by magnetic resonance force microscopy**
[J. Deichmüller](#)¹; K. Kartaschew¹; A. Rostas²; E. Schleicher²; S. Weber²; M. Havenith¹; ¹ Ruhr-Universität Bochum/D; ² Universität Freiburg/D
- P05-05 **Hyperfine structure in the IR-spectrum of ammonia, NH₃**
[G. Seyfang](#)¹; ¹ ETH Zürich/CH
- P05-06 **Kinetics of carbon-dioxide hydrate formation**
S. Schulze¹; J. Kiefer¹; [B. Rathke](#)¹; ¹ Universität Bremen/D
- P05-07 **Vapor-liquid Equilibria (VLE) of binary imidazolium-based ionic liquid mixtures with volatile solvents**
[M. Stuckenholtz](#)¹; J. Kiefer¹; B. Rathke¹; W. Schröer¹; ¹ Universität Bremen/D
- P05-08 **Ionenmobilitäten: Bestimmung durch ESI/REMPI-IMS und Vergleich verschiedener Berechnungsmethoden**
[D. Riebe](#)¹; A. Erler¹; T. Beitz¹; H. Löhmannsröben¹; ¹ Universität Potsdam/D
- P05-09 **Investigation of the thickness- and wavelength- dependence of laser stratigraphy on Cu and Ni using LIBS**
[U. Pacher](#)¹; T. Nagy¹; E. Khaybulkina¹; W. Kautek¹; ¹ University of Vienna/A
- P05-10 ***In situ* studies of gold nanoparticle formation in microfluidic reactors**
[G. Tofighi](#)¹; T. Sheppard¹; G. Hofmann¹; G. Rinke¹; R. Dittmeyer¹; J. Grunwaldt¹; ¹ Karlsruhe Institute of Technology (KIT)/D;

- P05-11

On the polymerization efficiency of benzoin-type photoinitiator molecules by fs-TA spectroscopy, PLP-ESI-MS and TD-DFT

C. Schweigert¹; ¹ Karlsruhe Institute of Technology (KIT)/D
- P05-12

COMOTION - controlling the motion of large molecules and particles

D. Horke¹; S. Awe¹; Z. Huang¹; N. Roth¹; N. Teschmit¹; T. Ossenbrüggen¹; D. Gusa¹; J. Küpper¹; ¹ Deutsches Elektronen Synchrotron DESY, Hamburg/D

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Photoelectron spectra from optimally tuned TDDFT and Dyson orbital formalism

T. Moehle¹; S. Bokarev¹; G. Grell¹; O. Kühn¹; ¹ University of Rostock/D;
- P06-02

Quantum-chemical calculations of metal-organic frameworks with open-shell adsorbates

E. Dietze¹; C. Herrmann¹; ¹ University of Hamburg/D
- P06-03

Hydrogen atom scattering from M(111) surfaces: molecular dynamics simulations on a full-dimensional EMT Potential Energy Surface

M. Kammeler¹; S. Janke¹; D. Auerbach¹; A. Wodtke¹; A. Kandratsenka¹; ¹ Max-Planck-Institute for Biophysical Chemistry, Göttingen/D
- P06-04

Computation and optimization of complex formation thermodynamics by a solute-solute integral equation theory

F. Mrugalla¹; S. Kast¹; ¹ TU Dortmund/D
- P06-05

Transfer free energies between aqueous and nonaqueous phases from an integral equation-based quantum solvation model

N. Tielker¹; D. Tomazic¹; S. Kast¹; ¹ TU Dortmund/D
- P06-06

Isomerization reaction kinetics in 2-methyltetrahydrofuran oxidation

P. Parab¹; N. Sakade²; Y. Sakai²; R. Fernandes³; K. Heufer¹; ¹ RWTH Aachen University/D; ² University of Fukui/J; ³ Physikalisch Technische Bundesanstalt (PTB), Braunschweig/D

Solids and Nano-sized Matter

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Imaging of gap plasmons and surface plasmon quenching in Au and Ag tip-sample-systems with cathodoluminescence

M. Grüßer¹; X. Ma¹; R. Schuster¹; ¹ Karlsruhe Institute of Technology (KIT)/D
- P07-02

Synthesis and control of emission properties of highly luminescent In(Zn)P/GaP/ZnS quantum dots

C. Meerbach¹; C. Rengers¹; M. Adam¹; N. Gaponik¹; A. Eychmüller¹; ¹ TU Dresden/D
- P07-03

Determination of the dimensions and extinction coefficient of CdSe seeded CdS nanorods through their UV/Vis spectra

P. Adel¹; J. Bloh¹; D. Hinrichs¹; T. Kodanek¹; D. Dorfs¹; ¹ Universität Hannover/D
- P07-04

The creation of highly emissive green - to - red Cu - In - Zn - S/ZnS core/shell quantum dots

J. Lox¹; M. Adam¹; T. Erdem²; H. Demir²; N. Gaponik¹; A. Eychmüller¹; ¹ TU Dresden/D; ² Bilkent University, Ankara/TR
- P07-05

Modification of binary semiconductor nanorods by site-selective growth of a heterojunction

F. Enders¹; K. Boldt¹; ¹ Universität Konstanz/D
- P07-06

Synthesis and spectroscopy of gold nanoclusters with different surface modifications

T. Hadler¹; T. Kipp¹; A. Mews¹; ¹ University of Hamburg/D
- P07-07

Optical and theoretical investigation of spectral diffusion of CdSe/CdS-Dotrods

S. Lohmann¹; C. Strelow¹; T. Kipp¹; A. Mews¹; ¹ University of Hamburg/D
- P07-08

Studies on the twinning effects during the self-assembly of silver nanoparticles into supercrystals

A. Reichhelm¹; D. Haubold¹; A. Eychmüller¹; ¹ TU Dresden/D
- P07-09

Development of a new nanostructured i-Sb₂S₃ / p-NiO junction photoelectrode

J. Schneider¹; Y. Wu¹; M. Barr³; L. Santinacci²; J. Bachmann¹; ¹ Universität Erlangen-Nürnberg, Erlangen/D; ³ Aix Marseille Université/F; ³ CNRS and Aix Marseille Université/F
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Influence of the modification on the initiation potential of nanoscale ZnO

M. Schmitt¹; ¹ Saarland University, Saarbrücken/D

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The formation of alkali ion beams from MAISi₂O₆ by thermionic emission

S. Schuld¹; M. Schäfer¹; K. Weitzel¹; ¹ Universität Marburg/D
- P07-12

Synthesis and characterization of CdSe/CdS nanorod decorated silica-coated plasmonic platinum nanoparticles

F. Lübke¹; ¹ Universität Hannover/D
- P07-13

Mechanism of gold nanoparticle growth in organic solvents

T. Redder¹; P. Witthöft¹; A. Mews¹; ¹ University of Hamburg/D
- P07-14

Shape-controlled Synthesis of Photoactive Two Dimensional SnS Nanosheets

M. Kobylinski¹; A. Mews¹; ¹ University of Hamburg/D
- P07-15

Simulations of alloying processes in nanoparticle assemblies

D. Lenz¹; T. Lorenz¹; J. Joswig¹; ¹ TU Dresden/D
- P07-16

Synthesis of tinsulfide-nanosheet networks via metal-organic chemical vapor deposition

C. Ruhmlied¹; A. Mews¹; ¹ University of Hamburg/D
- P07-17

Aerogel from CdSe and CdSe/CdS nanoplatelets

S. NASKAR¹; ¹ Universität Hannover/D
- P07-18

Combined local electrical and optical probes of individual Semiconductor nanostructures

A. Kolditz¹; ¹ University of Hamburg/D
- P07-19

Amine stabilized Au NP's for catalytic applications

L. Mohrhuse¹; M. Osmic¹; J. Kolny-Olesiak¹; K. Al-Shamery¹; ¹ University of Oldenburg/D
- P07-20

Versatile fabrication of voluminous nanocrystal aerogels

A. Freytag¹; N. Bigall¹; ¹ Universität Hannover/D
- P07-21

Embedding nonpolar quantum Dots into ionic matrices

C. Guhrenz¹; A. Benad¹; C. Bauer¹; M. Adam¹; J. Lox¹; C. Ziegler¹; N. Gaponik¹; A. Eychmüller¹; ¹ TU Dresden/D
- P07-22

Surface phenomena of metal nanowire networks as transparent electrodes for organic solar cells

L. Sonntag¹; ¹ TU Dresden/D
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Impact of redox-active molecules on the fluorescence of carbon nanotubes

E. Polo¹; ¹ Universität Göttingen/D
- P07-24

Localized surface plasmon resonance of Au-ITO heterodimers prepared by colloid chemistry

T. Mohamed¹; D. Dorfs¹; ¹ Universität Hannover/D
- P07-25

Influence of chloride ions on the shape and nucleation of CdS and CdSe on metal nanoparticles

D. Hinrichs¹; ¹ Universität Hannover/D
- P07-26

Assembly of shape-controlled semiconductor nanocrystals

L. Klepzig¹; P. Jan¹; N. Bigall¹; ¹ Universität Hannover/D
- P07-27

Improvement of photostability of silica covered CdSe/CdS-Dot/Rods through surface attached AuNPs-Layer

E. Kröger¹; ¹ University of Hamburg/D

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- P08-01

Internal complexation within starlike copolymers: influence of topology and composition

P. Hebbeker¹; A. Steinschulte¹; F. Plamper¹; S. Schneider¹; ¹ RWTH Aachen/D
- P08-02

Gas permeation through carbon nanomembranes

A. Beyer¹; V. Chinaryan¹; S. Shishatskiy²; J. Wind²; X. Zhang¹; H. Vieker³; P. Angelova³; V. Abetz²; A. Götzhäuser¹; ¹ University of Bielefeld/D; ² Helmholtz-Zentrum Geesthacht (HZG)/D; ³ CNM Technologies GmbH, Bielefeld/D
- P08-03

Polymer loops and tails attached to a surface, a dissipative particle dynamics study

M. Jehser¹; S. Eisenhaber¹; G. Zifferer¹; ¹ Universität Wien/A
- P08-04

Shielding effects in surface initiated polymerization studied by Dissipative Particle Dynamics (DPD)

S. Eisenhaber¹; M. Jehser¹; G. Zifferer¹; ¹ University of Vienna/A
- P08-05

Structure and time-dependent self-diffusion in binary mixtures of charge-stabilized colloidal suspensions

F. Ziegert¹; J. Wagner¹; ¹ Universität Rostock/D

- P08-06 **Detection of particle interaction in polydisperse highly concentrated polymer suspensions by Photon Density Wave spectroscopy**
L. Bressel¹; S. Pfuhl²; O. Reich¹; ¹ University of Potsdam and innoFSPEC, Potsdam/D; ² University of Potsdam/D
- P08-07 **Combination of fiber-optical methods for in-line multi-parameter analysis of the PNIPAm switching processes**
P. Werner¹; ¹ University of Potsdam and innoFSPEC, Potsdam/D

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X. Li¹; J. Paier¹; ¹ Humboldt-Universität zu Berlin/D
- P09-02 **Formaldehyde adsorption on the rutile TiO₂(110) surface probed by IR spectroscopy**
X. Yu¹; C. Yang¹; F. Bebensee¹; A. Nefedov¹; Z. Zhang²; Q. Ge³; Z. Dohnálek⁴; Y. Wang¹; C. Wöll¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Baylor University, Waco, TX/USA; ³ Southern Illinois University, Carbondale, IL/USA; ⁴ Pacific Northwest National Laboratory, Richland, WA/USA
- P09-03 **Microcalorimetric measurement of double layer charging in ionic liquids**
J. Lindner¹; S. Frittmann¹; F. Endres²; R. Schuster¹; ¹ Karlsruhe Institute of Technology (KIT)/D; ² TU Clausthal/D
- P09-04 **Structure dependent anchoring and thermal stability of organic molecules on atomically-defined oxide surfaces: phthalic acid on Co₃O₄(111), CoO(100) and CoO(111)**
T. Xu¹; M. Schwarz¹; K. Werner¹; S. Mohr¹; M. Amende¹; J. Libuda¹; ¹ Universität Erlangen-Nürnberg, Erlangen/D
- P09-05 **LiCoO₂-electrolyte interaction studied by surface science methods**
T. Späth¹; R. Hausbrand¹; W. Jaegermann¹; ¹ TU Darmstadt/D
- P09-06 **Relaxation dynamics and electron-transfer kinetics investigation on electrode|self-assembled monolayer|ionic liquid interfaces using electrochemical impedance spectroscopy**
N. Vargas-Barbosa¹; B. Roling¹; ¹ Universität Marburg/D
- P09-07 **Investigation of the interface of immiscible liquids by fluorescence light under microfluidic conditions**
H. Fischer¹; E. Antonsson¹; E. Rühl¹; ¹ Freie Universität Berlin/D
- P09-08 **Scattering of highly vibrationally excited NO from Ge(111)**
S. Meyer¹; B. Krüger¹; A. Wodtke¹; T. Schäfer¹; ¹ Universität Göttingen/D
- P09-09 **Vibrational energy pooling in multilayer CO on NaCl(100) studied with nanosecond time resolution using a superconducting nanowire single photon detector**
L. Chen¹; D. Schwarzer¹; A. Wodtke¹; ¹ Max-Planck-Institute for Biophysical Chemistry, Göttingen/D
- P09-10 **Multi-quantum vibrational relaxation in highly vibrationally excited NO/surface scattering: Influence of the surface**
B. Krüger¹; S. Meyer¹; A. Kandratsenka²; A. Wodtke¹; T. Schäfer¹; ¹ Universität Göttingen/D; ² Max-Planck-Institute for Biophysical Chemistry, Göttingen/D
- P09-11 **Energy transfer in collisions of highly vibrationally excited NO with vanadium dioxide surfaces**
A. Meling¹; B. Krüger¹; T. Schäfer¹; I. Rahinov²; A. Wodtke¹; ¹ Universität Göttingen/D; ² The Open University of Israel, Tel Aviv/IL
- P09-12 **Models systems for molecular energy storage: norbornadiene on Pt(111) and anchored to an atomically-defined cobalt oxide surface**
M. Schwarz¹; S. Mohr¹; T. Xu¹; O. Brummel¹; K. Werner¹; K. Civalé¹; T. Döpfer¹; U. Bauer¹; P. Bachmann¹; D. Besold¹; C. Papp¹; H. Steinrück¹; A. Görling¹; J. Bachmann¹; A. Hirsch¹; J. Libuda¹; ¹ Universität Erlangen-Nürnberg, Erlangen/D
- P09-13 **Quenching electronically and vibrationally excited carbon monoxide at metal surfaces using velocity controlled molecular beams**
R. Wagner¹; A. Meling¹; T. Schäfer¹; A. Wodtke¹; ¹ Universität Göttingen/D
- P09-14 **Fine structure in IR spectra of high quality CO₂ ultrathin films**
J. Vogt¹; ¹ University of Magdeburg/D
- P09-15 **Direct scattering of formaldehyde from the Au(111) surface**
B. Park¹; B. Krüger¹; S. Meyer¹; A. Wodtke¹; T. Schäfer¹; ¹ Universität Göttingen/D
- P09-16 **Time-resolved IR spectroscopy during interfacial electrochemical reactions of organic corrosion inhibitors**
Y. Chen¹; ¹ Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D

- P09-17 ***In-situ* IRAS studies of Tetraphenylporphyrins on Co₃O₄(111)/Ir(100)**
S. Mohr¹; K. Werner¹; M. Schwarz¹; M. Amende¹; T. Doepper¹; A. Goerling¹; J. Libuda¹; ¹ Universität Erlangen-Nürnberg, Erlangen/D
- P09-18 **The vanadium oxide monolayer on CeO₂(111) studied by density functional theory**
C. Penschke¹; J. Paier¹; J. Sauer¹; ¹ Humboldt-Universität zu Berlin/D
- P09-19 **Direct growth of patterned graphene**
A. Turchanin¹; ¹ Universität Jena/D
- P09-20 **Scattering HCl from Au(111): vibrational excitation probabilities and dissociative adsorption**
J. Geweke¹; P. Shirhatti¹; C. Steinsiek²; C. Bartels³; I. Rahinov⁴; A. Wodtke¹; ¹ Max-Planck-Institute for Biophysical Chemistry, Göttingen/D; ² Universität Göttingen/D; ³ Universität Freiburg/D; ⁴ Open University of Israel, Tel Aviv/D
- P09-21 **Electrostatic interactions and ligand effects at ionic-liquid modified interfaces: Co-adsorption of [EMIM][OTf] and CO on Pd(111)**
T. Bauer¹; S. Mehl¹; O. Brummel¹; K. Pohako-Esko¹; P. Wasserscheid¹; J. Libuda¹; ¹ Universität Erlangen-Nürnberg, Erlangen/D
- P09-22 **Ab initio molecular dynamics simulations of CO/NO scattering from Au(111)**
J. Altschäffel¹; A. Kandratsenka¹; A. Wodtke¹; ¹ Universität Göttingen/D
- P09-23 **Monitoring oxide layer growth on manganese electrodes, by *in-situ* spectroscopic ellipsometry and raman spectroscopy**
M. Rabe¹; A. Sarfraz¹; A. Erbe¹; ¹ Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D
- P09-24 **H at Au(111): an accurate full-dimensional potential energy surface**
S. Janke¹; A. Kandratsenka¹; Y. Dorenkamp¹; H. Jiang¹; O. Bünermann¹; D. Auerbach¹; A. Wodtke¹; ¹ University of Göttingen/D
- P09-25 **The effect of solvent and interfacial field affect on switching of a nitrospiropyran self-assembled monolayer at the solid/liquid interface**
T. Garling¹; Y. Tong¹; R. Campen¹; ¹ Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D
- P09-26 **Associative desorption of hydrogen from metal surfaces**
S. Kaufmann¹; Q. Shuai¹; D. Schwarzer¹; D. Auerbach¹; A. Wodtke¹; ¹ Max-Planck-Institute for Biophysical Chemistry, Göttingen/D
- P09-27 **CO adsorption on Pt₃Ti(111) studied by IRRAS and XPS**
L. Schöttner¹; M. Moors²; F. Bebensee³; A. Nefedov³; Y. Wang³; C. Wöll³; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Forschungszentrum Jülich/D; ³ Karlsruhe Institute of Technology (KIT)/D
- P09-28 **Reactivity of CO on sulfur-passivated graphene-supported palladium nanocluster arrays**
E. Düll¹; ¹ Universität Erlangen-Nürnberg, Erlangen/D
- P09-29 **A new thin film fabrication technique by interconnecting nanoparticles via tetrazole-complexes**
A. Wolf¹; C. Rengers¹; S. Voitekhovich²; V. Lesnyak¹; N. Gaponik¹; A. Eychmüller¹; ¹ TU Dresden/D; ² Belarusian State University, Minsk/BY
- P09-30 **Self-assembling amphiphilic fluorophores: *in-situ* monitoring and photonic characterization**
M. Hupfer¹; ¹ Universität Jena/D
- P09-31 **Photo-manipulation of the surface tension anisotropy at a liquid-crystal/ITO-glass interface**
A. Eremin¹; H. Nadasi¹; R. Stannarius¹; ¹ Universität Magdeburg/D

Biophysical Chemistry

- P10-01 **Molecular recognition in the organic corona around nanoparticles and applications to biosensing**
S. Kruss¹; ¹ Universität Göttingen/D
- P10-03 **Development of a label-free fiber optical biosensor based on etched fiber-Bragg-gratings**
S. Schulze¹; C. Hille¹; ¹ Universität Potsdam/D
- P10-04 **High-resolution femtosecond FT2D-IR spectroelectrochemistry**
J. Schmidt-Engler¹; Y. El Khoury¹; L. van Wilderen¹; J. Bredenbeck¹; ¹ Universität Frankfurt, Frankfurt/D
- P10-05 **Noninvasive, label-free analysis of stimulus-induced cellular activity using Raman spectroscopic imaging**
A. Post¹; C. Hille¹; ¹ Universität Potsdam/D

P10-06 **Liquid-liquid phase separation in therapeutic monoclonal antibody systems**
[P. Garidel](#)¹; ¹ Universität Halle-Wittenberg, Biberach/D

P10-07 **Validation and comparison of biomolecular force fields regarding structural properties and binding affinities of cyclodextrins**
[J. Gebhardt](#)¹; N. Hansen¹; ¹ University of Stuttgart/D

P10-08 **Signal mechanism of integrin α V β 3**
W. Langel¹; [M. Kulke](#)¹; ¹ Universität Greifswald/D

P10-09 **Probing the function of calmodulin adsorbed on and embedded in polyelectrolyte multilayers**
[S. Cinar](#)¹; C. Czeslik¹; ¹ TU Dortmund/D

P10-10 **Activation volumes of enzymes at polyelectrolyte brushes**
[A. Levin](#)¹; C. Czeslik¹; ¹ TU Dortmund/D

P10-11 **Cosolvent and crowding effects on the temperature and pressure stability of monomeric actin**
[P. Schummel](#)¹; R. Winter¹; ¹ TU Dortmund/D

P10-12 **Penetration of dexamethasone in human skin investigated by X-ray spectromicroscopy**
[K. Yamamoto](#)¹; A. Klossek¹; R. Flesch¹; F. Rancan²; M. Weigand³; I. Bykova³; M. Bechtel³; P. Patoka¹; G. Ulrich¹; S. Ahlberg²; A. Vogt²; U. Blume-Peytavi²; P. Schrade²; S. Bachmann²; M. Schäfer-Korting²; E. Rühl¹; ¹ Freie Universität Berlin/D; ² Charite Universitätsmedizin Berlin/D; ³ Max-Planck-Institut für Intelligente Systeme, Stuttgart/D

P10-13 **CRMP2: switching structures**
[D. Möller](#)¹; C. Lillig¹; M. Gellert¹; N. Geist¹; W. Langel¹; ¹ Universität Greifswald/D

P10-14 **Efficient energy transfer as switching mechanism for super-resolution microscopy**
[A. Haderspeck](#)¹; D. Brox¹; D. Herten¹; ¹ University of Heidelberg/D

P10-15 **Allostery in PDZ3: azidohomoalanine as site-specific probe for IR spectroscopy**
[K. Eberl](#)¹; P. Quoika¹; H. Müller-Werkmeister¹; J. Löffler¹; M. Essig¹; J. Bredenbeck¹; ¹ University of Frankfurt/D

P10-16 **Shedding light on plasma-bacteria interaction using vibrational microspectroscopy**
[K. Kartaschew](#)¹; S. Baldus¹; F. Kogelheide¹; M. Mischo¹; J. Lackmann¹; P. Awakowicz¹; M. Havenith¹; ¹ Ruhr-Universität Bochum/D

P10-17 **Understanding the primary steps of light-induced signal propagation of an artificial LOV2-Rac1 photoswitch**
[I. Stambolic](#)¹; ¹ University of Regensburg/D

P10-18 **The flavin photochemistry in a LOV domain is tuned and controlled by the protein environment**
[K. Magerl](#)¹; ¹ Universität Regensburg/D

P10-19 **Targeted delivery of aptamer- and antibody-conjugated AuNPs to Interleukin-6 receptor-carrying cells**
[L. Prisner](#)¹; N. Bohn¹; M. Bendig¹; A. Mews¹; ¹ Universität Hamburg/D

P10-20 **Effect of the N-terminal Helix and Nucleotide-loading on the membrane and effector binding of the GTPases Arl2 and Arl3**
S. Kapoor¹; E. Fansa²; S. Möbitz³; S. Ismail⁴; R. Winter³; A. Wittinghofer²; [K. Weise](#)³; ¹ TU Dortmund and Max Planck Institute of Molecular Physiology, Dortmund/D; ² Max Planck Institute of Molecular Physiology, Dortmund/D; ³ TU Dortmund/D; ⁴ Max Planck Institute of Molecular Physiology and CR-UK Beatson Institute, Glasgow/UK

P10-21 **Kinetics of drug release and mobility in healthy and osteoporotic rat bone**
[M. Rohnke](#)¹; ¹ University of Giessen/D

P10-22 **Calculation of relative folding free enthalpies of amide-to-ester mutants of protein Pin1**
[D. Markthaler](#)¹; ¹ Universität Stuttgart/D

P10-23 **Counting LAT and SLP-76 in the T-cell antigen receptor proximal signaling microcluster**
[W. Chmielewicz](#)¹; S. Hänselmann¹; K. Yserentant¹; K. Grußmayer¹; D. Herten¹; ¹ Heidelberg University/D

P10-24 **Comparing azide and thiocyanate vibrational probes for infrared spectroscopy of proteins**
[M. Mikorski](#)¹; D. Kern-Michler¹; K. Eberl¹; L. van Wilderen¹; J. Bredenbeck¹; ¹ Universität Frankfurt/D

P10-25 **Pressure-induced effects on self-cleavage reaction of ribozyme catalysis: a molecular dynamics study**
[N. Kumar](#)¹; ¹ Ruhr-Universität Bochum/D

Catalysis	
P11-01	Oxygen chain structures and other forms of chemisorbed oxygen on gold-silver alloy surfaces: a DFT study L. Moskaleva ¹ ; T. Weiss ¹ ; M. Bäumer ¹ ; T. Klüner ² ; ¹ Universität Bremen/D; ² Universität Oldenburg/D
P11-02	Decomposition of formic acid on Pd-based surfaces H. Euchner ¹ ; ¹ Ulm University/D
P11-03	Computational methods for pure component decompositions with application to the rhodium catalyzed hydroformylation K. Neymeyr ¹ ; M. Sawall ¹ ; A. Jürß ¹ ; H. Schröder ¹ ; ¹ University of Rostock/D
P11-04	Formic acid dehydrogenation over Au/CeO₂ catalysts: theoretical DFT study J. Kucera ¹ ; A. Groß ¹ ; ¹ Ulm University/D
P11-05	Operando X-ray absorption and emission spectroscopy to understand reaction mechanisms in NO_x-removal catalysts T. Günter ¹ ; D. Doronkin ¹ ; A. Boubnov ¹ ; M. Casapu ¹ ; J. Grunwaldt ¹ ; J. Rudolph ² ; C. Jacob ² ; ¹ Karlsruher Institut für Technologie (KIT)/D; ² TU Braunschweig/D
P11-06	Nanoporous gold supported oxides as high-performance hydrogen production catalyst J. Shi ¹ ; A. Lackmann ¹ ; A. Wittstock ¹ ; M. Bäumer ¹ ; ¹ University of Bremen/D

Electrochemistry and Energy	
P12-01	Electroplating of polyurethane foams S. Keck ¹ ; A. Jung ¹ ; R. Hempelmann ¹ ; H. Natter ¹ ; ¹ Saarland University, Saarbrücken/D
P12-02	New catalyst supports for energy conversion prepared by surface modification of Graphene- and CNT-structures E. Oh ¹ ; ¹ Saarland University, Saarbrücken/D
P12-03	Characterization and improvement of the active materials in the vanadium redox flow battery K. Weißhaar ¹ ; H. Natter ¹ ; R. Hempelmann ¹ ; ¹ Saarland University, Saarbrücken/D
P12-04	Development of an improved state – of – charge indicator for the all – vanadium redox flow battery J. Geiser ¹ ; H. Natter ¹ ; R. Hempelmann ¹ ; ¹ Saarland University, Saarbrücken/D
P12-05	Perovskites containing protons, oxygen vacancies and holes: experiments and simulations for proton uptake and stoichiometry relaxation kinetics R. Zohourian Aboutorabi ¹ ; R. Merkle ¹ ; J. Maier ¹ ; ¹ Max Planck Institute for Solid State Research, Stuttgart/D
P12-06	Investigation of co-adsorption and side processes during underpotential deposition of Cu and Ag on Au(111) by electrochemical microcalorimetry S. Frittmann ¹ ; V. Halka ¹ ; R. Schuster ¹ ; ¹ Karlsruher Institut für Technologie (KIT)/D
P12-07	Designed architectures of electrode materials for advanced Li (Na)-ion batteries Y. Yu ¹ ; ¹ Max Planck Institute for Solid State Research, Stuttgart/D
P12-08	On the calculation of excess functions of electrolytes A. Maurer ¹ ; H. Krienke ² ; D. Horinek ² ; G. Schmeer ² ; ¹ University of Regensburg, Tirschenreuth/D; ² University of Regensburg/D
P12-09	Manganese oxides for the oxygen evolution reaction J. Doerfer ¹ ; J. Schuch ¹ ; B. Kaiser ¹ ; W. Jaegermann ¹ ; ¹ TU Darmstadt/D
P12-10	<i>In situ</i> method for efficient catalyst layer production with very low catalyst loading R. Engstler ¹ ; D. Durneata ¹ ; H. Natter ¹ ; R. Hempelmann ¹ ; ¹ Saarland University, Saarbrücken/D
P12-11	BaTiO₃ modifications for photochemical hydrogen evolution Y. Xiong ¹ ; ¹ Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr/D
P12-12	Long-term stability of silicon-poisoned La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-δ} SOFC-cathodes M. Perz ¹ ; E. Bucher ¹ ; A. Egger ¹ ; C. Gspan ² ; F. Hofer ² ; W. Sitte ¹ ; ¹ Montanuniversitaet Leoben/A; ² Graz University of Technology/A
P12-13	Development of a photocapacitor based on printed solar cells and super capacitors K. Anneser ¹ ; S. Braxmeier ¹ ; A. Baumann ¹ ; G. Reichenauer ¹ ; V. Dyakonov ² ; ¹ Bavarian Center for Applied Energy Research, Würzburg/D; ² University of Würzburg/D

- P12-14

Electron bombardment induced cation transport in an ion conducting glass
A. Hein¹; J. Wiemer¹; K. Weitzel¹; ¹ Universität Marburg/D
- P12-15

Sulfide electrolytes based on Glyme-Lithium salt mixtures for new battery systems
A. Bónsa¹; A. Appelhagen¹; J. Lehmann¹; R. Ludwig¹; ¹ University of Rostock/D
- P12-16

Electrochemical study of Si-nanodroplets deposited on graphite using a LPCVD process
K. Nimmrich¹; D. Klein¹; T. Bartoldus²; S. Cap¹; R. Schlögl¹; ¹ Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D; ² Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr/D
- P12-17

Development of electrocatalysts for alkaline water electrolysis
A. Surkus¹; M. Polyakov¹; N. Rockstroh¹; H. Junge¹; A. Martin¹; M. Beller¹; ¹ Leibniz-Institute for Catalysis, Rostock/D
- P12-18

Preparation of titanium dioxide thin films by atomic layer deposition applied on tandem solar cells for photoelectrochemical water splitting
T. Cottre¹; J. Ziegler¹; B. Kaiser¹; W. Jaegermann¹; ¹ TU Darmstadt/D

Industrial Applications

P13-01

Metrological support for LNG custody transfer and transport fuel applications
J. Rauch¹; K. Arrhenius²; M. Downey³; B. Giesekeing³; P. Eilts⁴; H. Ent⁵; O. Kerkhof⁵; J. Li⁵; P. Albo⁶; A. Lucassen¹; G. Nieuwenkamp⁵; M. Richter⁷; A. van der Veen⁵; ¹ Physikalisch-Technische Bundesanstalt (PTB), Braunschweig/D; ² SP Sveriges Tekniska Forskningsinstitut AB (SP), Borås/S; ³ National Physical Laboratory (NPL), Teddington/UK; ⁴ TU Braunschweig/D; ⁵ VSL Dutch Metrology Institute, Delft/NL; ⁶ Istituto Nazionale di Ricerca Metrologica (INRiM), Turin/D; ⁷ Ruhr-Universität Bochum/D

Thursday, 5 May 2016

19:30 – 22:00

Welcome Reception

(Tent)

Price: 10 € (incl. 19% VAT) nominal charge

Friday, 6 May 2016

9:30

Day trip to the artist’s colony in Ahrenshoop: art between the sea and the bodden
Meeting at 9:30 am in front of the main lecture hall, Ulmencampus
Registration necessary, max. 25 participants, Fee 25 €

12:30 – 13:30

Women’s Networking Lunch

(Haus 1, SR 021)

Lunch Speech:
Prof. Dr. Katharina Kohse-Höinghaus (Universität Bielefeld /D)
Price: 10 € (incl. 19% VAT) nominal charge
The number of participants is limited to 40.

The Bunsen Society invites all women to this third Women’s Networking Lunch at the Bunsentagung 2016 – it is a tradition now!

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.

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.

We are looking forward to seeing you at the Lunch!

Yvonne Joseph & Melanie Schnell

18:00 – 21:00

Poster Session & Poster Dinner

(Tent)

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.

Saturday, 7 May 2016

9:30

Sightseeing in Rostock
Meeting at 9:30 at Kröpeliner Tor/ Kröpelin Gate

Morning program: Walking tour in the city centre
Exhibition „State Security in the SED-Dictatorship“ in the historical site of the former prison and seat of the Minister of State Security (BStU), the Astronomical Clock at St. Mary’s Church
Registration necessary, max. 25 participants, Fee 8 €

REGISTRATION FEES¹⁾

Registration fees until 4 March 2016

Personal Members of the German Bunsen Society	180 €
Non-Members	255 €
Students ²⁾ (proof of status required, no Ph.D. students)	50 €
Accompanying Person ³⁾	65 €

Registrations after 4 March 2016 will be charged a 25 € late fee (except for accompanying person).

1) No VAT requested according § 4.21 USTG

2) Students enrolled in Bachelor and Master Courses only. Ph.D. students will be charged the regular registration fee.

3) Only participation to the Opening Ceremony, Opening Lecture and Welcome Dinner on 5 May 2016 and the Poster Session and Poster Dinner on 6 May 2016 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.

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 **13 April 2016**. 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 **13 April 2016**. 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, via the item “Accommodation”.

Participants should make their reservations with the hotel directly. Please provide the keyword “Bunsen/Bunsentagung” for a special rate. We highly recommend to book your accomodation as early as possible.

VENUE

Universität Rostock
Ulmencampus
Ulmestraße 69
18057 Rostock

HOW TO REACH THE VENUE

On the conference website www.bunsentagung.de, under the menu “Venue”, you’ll find a link to the route description to the University of Rostock as well as information on reduced fare railway tickets to DECHEMA events.

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

(Haus 1, SR 022)

Thursday, 5 May 2016	11:00 – 19:00
Friday, 6 May 2016	08:00 – 18:00
Saturday, 7 May 2016	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

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

Mrs. Carmen Weidner-Friedrich

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E-mail: geschaeftsstelle@bunsen.de

Internet: 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 available.

POSTER SESSION, POSTER DINNER AND POSTER AWARDS

Friday, 6 May 2016

18:00 – 21:00

Posters will be on display during the entire conference. There will also be a dedicated “Poster Session” on Friday, 6 May 2016 from 18:00-21:00. The session will be split between even poster numbers (from 18:00 to 19:30) and odd poster numbers (from 19:30 to 21:00). 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 morning between 8:30 and 10:50.

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 2017 for the main author.

The **Poster Award Ceremony** will take place during the **Closing Ceremony on Saturday 7 May 2016 at 16:00**.

Only authors present at the Closing Ceremony will be awarded.

GENERAL INFORMATION

KARRIEREFORUM (in German only)**Thursday, 5 May 2016****12:00 – 15:00** (Arno-Esch II)**Topic: Forschung nach der Promotion**

The “Karriereförum” is a symposium held annually organized by the Karriereförum working group of the German Bunsen Society. The symposium addresses mainly Ph.D. students at the end of their doctorate, postdocs and young scientists and provides a platform for the exchange and discussion of career-related issues.

The topic of this year’s forum is “Research after Ph.D.” and intends to high-light the variety of career opportunities within science, alternative to German universities, which are not familiar to the majority of the participants.

Please note, that – with the exception of the last talk – the “Karriereförum” will be held in German. **Admission is free, but online registration in advance is required.** Please tick the appropriate box on the online registration form.

Please note, that the “Karriereförum” will be in German.

Information material will also be available at the “Karriereförum” stand at the accompanying exhibition.

The “Mitgliederversammlung AG Karriereförum” will take place on Saturday during lunch break in Haus 1, SR 025.

Programm:

- | | |
|---------------|---|
| 12:00 – 12:10 | Eröffnung des Karriereförums durch die Sprecher:
Dr. Jan Porada (Universität Stuttgart), Dr. Aras Kartouzian (Technische Universität München) |
| 12:10 – 13:00 | Dr. Anne Schreiter (German Scholar Organization e.V. GSO, Berlin)
<i>Forschungskarriere mal anders: Perspektiven für Nachwuchswissenschaftler außerhalb deutscher Universitäten</i> |
| 13:00 – 13:20 | Pause |
| 13:20 – 14:10 | Dr. Oliver Lade (Clariant, Frankfurt)
<i>Anforderungen der zukunftsorientierten Spezialchemie an den physikalisch-chemischen Forscher in der Industrie</i> |
| 14:10 – 15:00 | Prof. Dr. Jan Lagerwall (University of Luxembourg)
<i>When coming home becomes visiting, and leaving becomes coming home: reflections on a globalized researcher's life</i> |

Detailed description of the speakers and the topics can be found on the website.

CHILD CARE

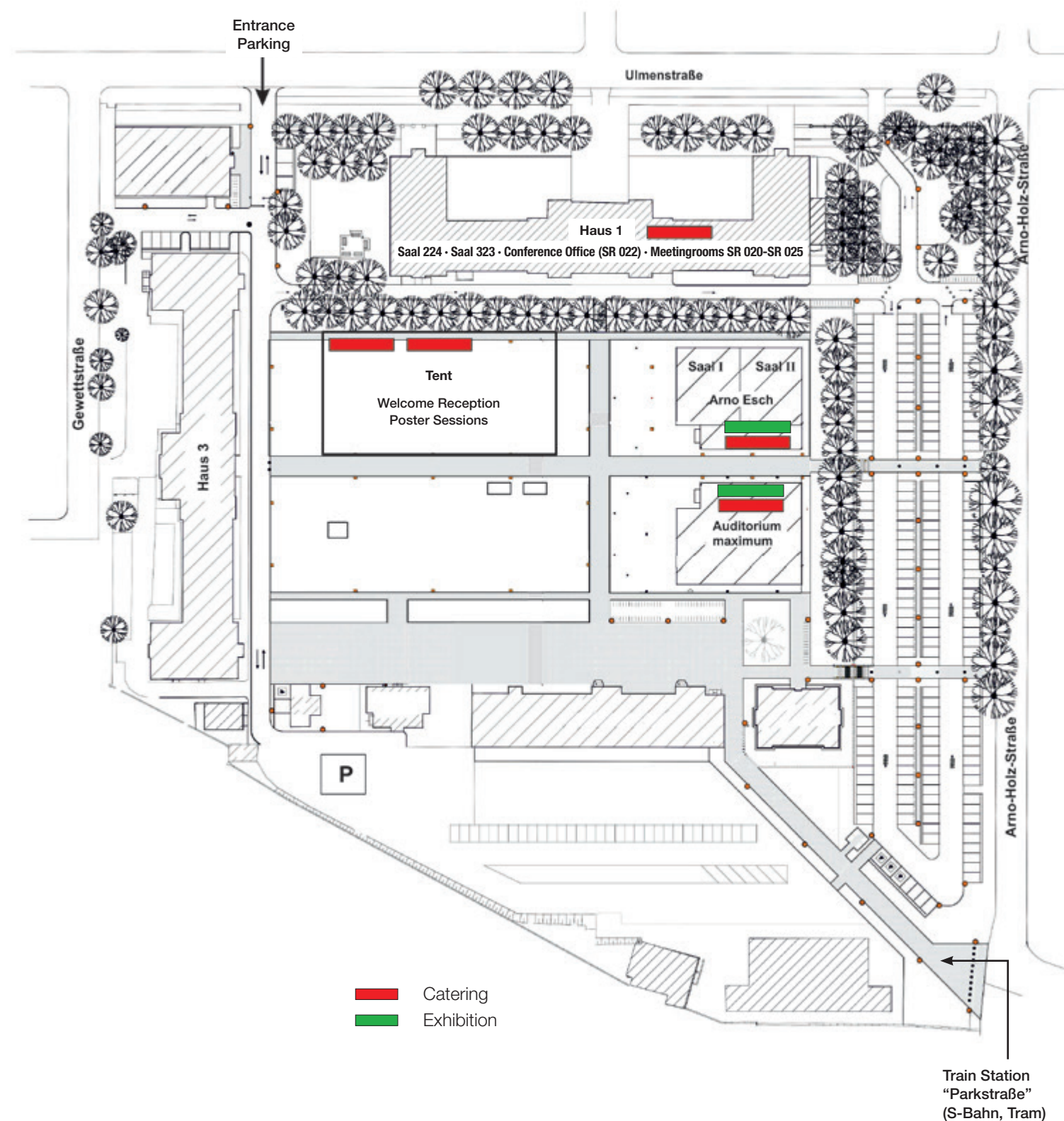
The Bunsentagung offers the opportunity for child care service to parents of small children during the event for a service charge of 10 €. Interested parents are requested to complete the form which can be found at www.bunsentagung.de/childcare2016 and send it to the congress office by 6 April 2016. A minimum number of 5 children is necessary. Parents will be informed whether the service can be offered after the deadline.

INTERNET SERVICE

Free internet access will be provided via the eduroam service (<https://www.eduroam.org>) for all participants during the conference. Online registration in advance is requested to use WLAN via other services.

More and regularly updated information on the conference is available at
www.bunsentagung.de

MAP





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