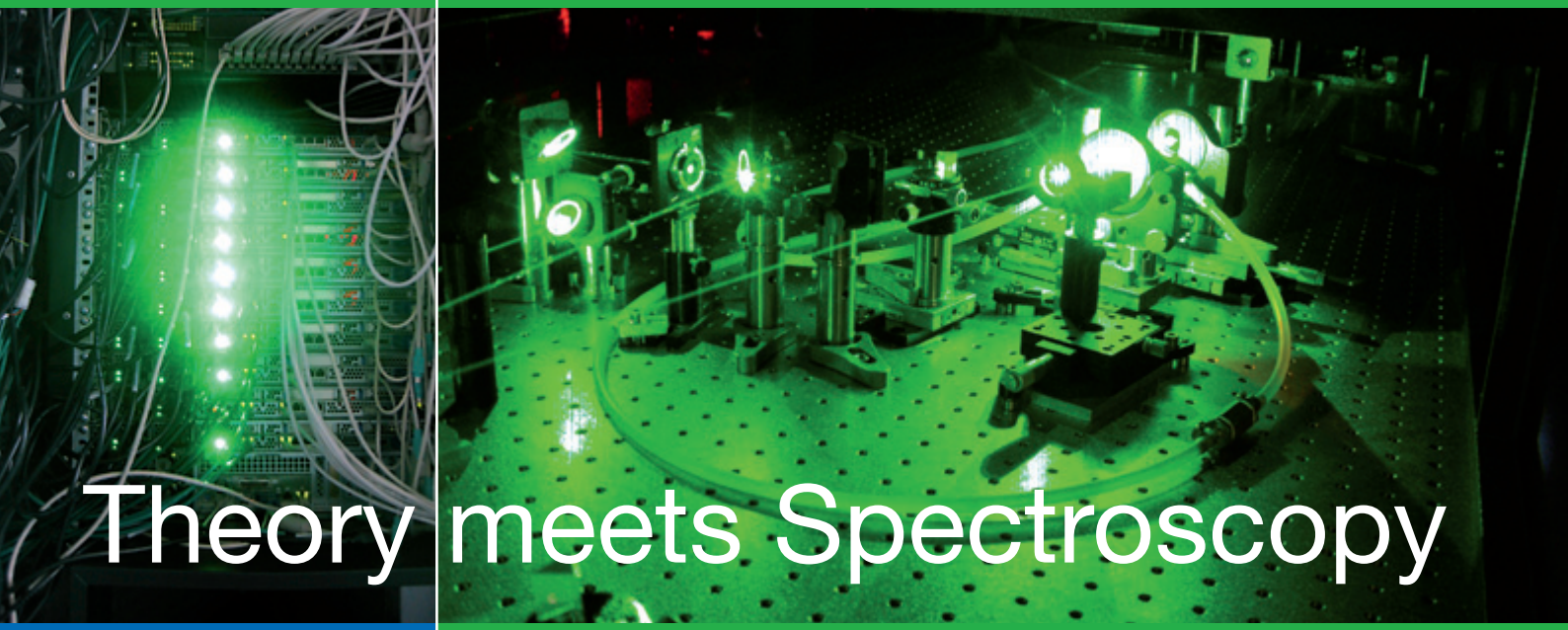
PROGRAMME

May 09 – 11, 2013 · Karlsruhe · Germany



BUNSENTAGUNG 2013

112th General Assembly of the German Bunsen Society for Physical Chemistry

Also featuring a special symposium “Electrochemical Interfaces”, an industrial symposium with accompanying exhibition, and the “Karriereforum”

Karlsruhe Institute of Technology

Division of Physical Chemistry · EuCheMS

www.bunsentagung.de

MAIN TOPIC:

“Theory meets Spectroscopy”

The main topic of the Bunsentagung 2013 focuses on state-of-the-art research in the fields of theoretical spectroscopy as well as molecular characterisation using experimental spectroscopy guided by quantum chemistry. This also includes recent advances in experimental techniques that probe molecules in gas and condensed phases under precisely defined/controlled conditions as well as new developments in describing such systems theoretically at a predictive level.

There is a long-standing research synergy between molecular spectroscopy and quantum chemistry. Both fields are interested in eigenstates and how these can be interconverted by electromagnetic radiation. In the last ten years, new experiments have increasingly been stimulated by computational predictions while theoretical approaches have often benefited from experimental benchmarks. This trend will accelerate further due to recent developments in both theory and spectroscopic measurement. Experimental advances include methods which allow for better-defined samples (e.g., mass and conformer selection of large molecular ions, ultralow temperature cooling schemes, surface immobilization methods, etc.) and their spectroscopic characterisation at highest frequency and time resolutions. This has in turn enabled spectroscopic probes and spectroscopic control of chemical change at unprecedented levels of precision – with ramifications for fields ranging from nanoscience and catalysis to photo- and biophysical chemistry. In the last decades, novel quantum-chemical methods have been developed at a breathtaking pace, and as such they continue to be developed further. Today, a large variety of spectra can be simulated, many spectroscopic properties can be computed, larger molecular systems can be treated than before (e.g., in the framework of density-functional theory), and an extreme accuracy can be achieved (e.g., using coupled-cluster theory for rotational spectroscopy). Advanced time-dependent methods have been developed as well as efficient computational models to describe surface-bound systems and molecules in condensed phases (e.g., QM/MM methods, embedding schemes, and molecular dynamics simulations). Much recent work has been concerned with predictive-level treatments of electronically excited states and (non-radiative) transitions.

The main topic of the 112th Bunsentagung seeks to highlight the growing importance of the synergetic interplay between theory and spectroscopy in advancing the field of molecular chemical physics in the age of Moore´s law. As rapidly increasing computational resources become available, some areas of experiment are already being supplanted by predictive-level theoretical spectroscopy. Other areas of experimental spectroscopy, concerned with more complex molecular systems, can presently help to further develop theory by providing benchmarks. Finally, certain areas of molecular spectroscopy (e.g., under extreme conditions) will remain inaccessible to accurate computational prediction for quite a while yet. Nevertheless, even here useful physical insight will result from quantum-chemical model calculations.

The talks of this symposium are intended to illustrate and further encourage this synergy between modern spectroscopy and state-of-the-art quantum-chemical calculations – in terms of examples ranging from molecules in gas-phase, through surface-bound to interacting-in-condensed-phase.

PROGRAMME COMMITTEE

Wolfgang Domcke	TU München, Garching/D
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Karin Fink	Karlsruhe Institute of Technology/D
Jürgen Gauß	University of Mainz/D
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Manfred Wilhelm	Karlsruhe Institute of Technology/D
Christof Wöll	Karlsruhe Institute of Technology/D
Rudolf Zentel	University of Mainz/D

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Jürgen Gauß	University of Mainz/D
Manfred Kappes	Karlsruhe Institute of Technology/D
Willem Klopper	Karlsruhe Institute of Technology/D

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Patrick Weis	Karlsruhe Institute of Technology/D
Christof Wöll	Karlsruhe Institute of Technology/D

HOST

Deutsche Bunsen-Gesellschaft für Physikalische Chemie e.V.
German Bunsen Society for Physical Chemistry
Theodor-Heuss-Allee 25
60486 Frankfurt am Main/D
Phone: +49 (0)69 7564-621
Fax: +49 (0)69 7564-622
E-Mail: woehler@bunsen.de
Internet: www.bunsen.de

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If you are interested in either exhibiting or sponsoring, please contact the local organisers directly (**bunsen2013@ipc.kit.edu**).

LIST OF EXHIBITORS (as of February 10, 2013)

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You can also support the conference via a direct donation to the German Bunsen Society. Please contact Mrs Erika Wöhler (woehler@bunsen.de) for additional information.

MEETINGS OF THE GERMAN BUNSEN SOCIETY

Thursday, May 9, 2013	
09:00 – 11:00	**Vorstandssitzung*** (nur auf Einladung)
09:00 – 11:00	**Sitzung der Unterrichtskommission*** (nur auf Einladung)
09:00 – 11:00	**Sitzung der Themenkommission*** (nur auf Einladung)
11:00 – 14:00	**Sitzung des Ständigen Ausschusses*** (nur auf Einladung)
11:30 – 14:45	**Karriereforum*** Thema: „Anträge, Stipendien, Nachwuchsgruppe – Fördermöglichkeiten für Nachwuchswissenschaftler“
15:00 – 16:15	**Ordentliche Mitgliederversammlung*** (nur für Mitglieder der DBG)

*in German only

Thursday, May 9, 2013

11:30	**KARRIEREFORUM*** – Room: CRIEGEE (see page 43)
15:00	**Ordentliche Mitgliederversammlung*** (nur für Mitglieder der DBG)

* in German only

	AUDIMAX
16:30	**OPENING CEREMONY**
18:00	**OPENING LECTURE: M. Ashfold**
19:30	**WELCOME RECEPTION** – Room: Festsaal Studentenwerk KIT (see page 39)

Friday, May 10, 2013

8:30 - 9:15	AUDIMAX	PLENARY LECTURE: **D. Marx** – *Chair: M. Peuckert*					
	AUDIMAX	HÖRSAAL I	CRIEGEE	HÖRSAAL II	AOC 101	HÖRSAAL III	NEUER CHEMIEHÖRSAAL
	Theory meets Spectroscopy (main topic)	Interfaces	Industrial Symposium	Gaseous State	Biophysical Chemistry	Joint Session Solid State/ Electrochemical Interfaces	Physical-Chemical Methods
Chair:	*M. Kappes*	*Y. Joseph*	*M. Wilhelm*	*M. Olzmann*	*U. Nienhaus*	*R. Schuster*	*E. Goos*
9:20 - 9:40	FULL LECTURE **T. Rizzo**	T. Lenzer	P. Zänker	M. Gaffga	J. Seeliger	FULL LECTURE **B. Roling**	T. Benzler
9:40 - 10:00		C. Raschpichler		N. Schirmel	A. Meister		P. Patoka
10:00 - 10:20	C. Baldauf	A. Sarfraz	M. Schmidt	B. Kieling	A. Hädicke	J. Popovic	M. Hippler
10:20 - 10:40	K. Schwing	F. Heib		J. Giegerich	S. Kapoor	P. Bottke	J. Bredenbeck
10:40 - 11:00	Coffee Break						
Chair:	*J. Sauer*	*J.P. Hofmann*	*M. Wilhelm*	*J.-U. Grabow*	*G. Jung*	*B. Roling*	*J. Bredenbeck*
11:00 - 11:20	FULL LECTURE **B. Mennucci**	FULL LECTURE **G. Friedrichs**	T. Hofe	S. Trippel	M. Drescher	A. Kuhn	X. Stammer
11:20 - 11:40				T.M. Bernhardt	T. Kottke	D. Samuelis	C. Hess
11:40 - 12:00	C. Allolio	M. Pedio	N. Nestle	J.R. Meyer	A. Garrone	N. Ohmer	E. Barsch
12:00 - 12:20	A. Klamt	S. Waschke	I. Vittorias	D. Schooss	[illegible]ingart	M. Kaus	M. Eichelbaum
12:20 - 13.30	Lunch Break						
13:30 - 14:15	AUDIMAX	PLENARY LECTURE: **T. Brixner** – *Chair: M. Quack*					
	Theory meets Spectroscopy (main topic)	Interfaces	Industrial Symposium	Gaseous State	Biophysical Chemistry	Electrochemical Interfaces	Physical-Chemical Methods
Chair:	*M. Quack*	*K. Al-Shamery*	*O. Deutschmann*	*A. Fielicke*	*T. Kottke*	*A. Kuhn*	*M. Hippler*
14:20 - 14:40	F. Kollipost	A. Kerth	T. Mäurer	G. Lendvay	FULL LECTURE **M. Havenith**	R. Chen	F. Stolz
14:40 - 15:00	H. Köppel	M. Laurin		A. Lucassen		M. Mutke	C. Riehn
15:00 - 15:20	N. Heine	B. Mosebach	M. Votsmeier	FULL LECTURE **T. Zeuch**	S. Heuke	B. Horstmann	A. Vollmer
15:20 - 15:40	M. Stein	F. Leroy	P.A. Neff		F. Schinle	S.L. Koch	N. Olichwer
15:40 - 16:00	Coffee Break						
	Theory meets Spectroscopy (main topic)	Interfaces	Industrial Symposium	Solid State	Biophysical Chemistry	Electrochemical Interfaces	Physical-Chemical Methods
Chair:	*W. Klopper*	*C. Wöll*	*M. Peuckert*	*D. Samuelis*	*B. Luy*	*R. Schuster*	*A. Köhn*
16:00 - 16:20	FULL LECTURE **J.F. Stanton**	C. Azucena	H.J. Limbach	R.A. De Souza	M. Mischo	FULL LECTURE **P. Allongue**	F.M. Kuhn
16:20 - 16:40		C. Amiri Naini		J. Keppner	A. Fogarty		P. Goel
16:40 - 17:00	S. Thorwirth	L. Schade	J. Lacayo	R. Merkle	C. Czeslik	E. Steyskal	T. Körzdörfer
17:00 - 17:20	N.O.B. Lüttschwager	O. Armbruster		R. Dolle	A.-M. Kreuziger	A. Lahiri	S. Irle
17:20 - 17:40	G. Rauhut	W. Kautek	M. Luft	G. Gregori	S.C. Salmen	F. Theil	A. Bande
17:40 - 18:00	M. Bauer	C. Graf		P. Gaczynski	M. Hanke	W.E. Gomes	M. Lewerenz
18:00 - 22:00	**Poster Session** (see page 42)						

Saturday, May 11, 2013

8:30 - 9:15	AUDIMAX	PLENARY LECTURE: **F. Neese** – *Chair: W. Domcke*					
	AUDIMAX	HÖRSAAL I	CRIEGEE	HÖRSAAL II	AOC 101	HÖRSAAL III	NEUER CHEMIEHÖRSAAL
	Theory meets Spectroscopy (main topic)	Interfaces	Theory meets Spectroscopy (main topic)	Solid State	Soft Matter	Electrochemical Interfaces	Hot Topics
Chair:	*W. Domcke*	*A. Turchanin*	*A. Bande*	*E. Bucher*	*C. Czeslik*	*B. Horstmann*	*M. Quack*
9:20 - 9:40	FULL LECTURE **M. Kawai**	A. Hertwig	B. Helmich	A.K. Opitz	S. Seiffert	FULL LECTURE **M. Rohwerder**	S. Albert
9:40 - 10:00		Y. Joseph	R.A. Mata	A. Düvel	B. Engels		P. Kraus
10:00 - 10:20	C. Ochsenfeld	H. Gliemann	M.-O. Winghart	D. Budina	L. Chiappisi	A. Erbe	P.M. Clawin
10:20 - 10:40	Coffee Break						
Chair:	*M.Schnell*	*W. Kautek*	*G. Rauhut*	*G. Gregori*	*S. Seiffert*	*C. Roth*	*R. Schäfer*
10:40 - 11:00	FULL LECTURE **C. Puzzarini**	B. Kern	D. Friese	M. Springborg	E. Voyiatzis	FULL LECTURE **T. Jacob**	J.P. Hofmann
11:00 - 11:20		J.M. Gottfried	R. Ludwig	B. Herd	S. Eisenhaber		N. Rühl
11:20 - 11:40	J.-U. Grabow	C. Heine	M. Thomas	H.W. Pereira de Carvalho	J. Liu	P.U. Biedermann	K.-H. Ernst
11:40 - 12:00	V.A. Shubert	J. Behler	L. Horny	T. Hertel	M. Stadler	L. Wittern	P. Angelova
12:00 - 12:20	H. Mouhib	S. Schauermann	O. Steinhauser	M. Müller	N. Kapernaum	H. Natter	S. Nayak
12:20 - 13:30	Lunch Break						
13:30 - 14:15	AUDIMAX	PLENARY LECTURE: **M. Wolf** – *Chair: J. Gauß*					
	Theory meets Spectroscopy (main topic)		Theory meets Spectroscopy (main topic)	Solid State	Liquid State	Electrochemical Interfaces	Joint Session DFG Funding / DBG Awards
Chair:	*J. Gauß*		*K. Fink*	*M. Springborg*	*W. von Rybinski*	*R. Merkle*	*M. Peuckert*
14:20 - 14:40	FULL LECTURE **B. Abel**		A. Kelterer	M. Scheuermann	K.R. Siefermann	F. Yang	J. Kowol-Santen K. Winkler
14:40 - 15:00			A. Köhn	H. Schlicke	G. Schwaab	S. Schulze	
15:00 - 15:20	A. Fielicke		T.N.V. Karsili	J. Kolny-Olesiak	P. Stange	V. Metlenko	AWARD LECTURE **Bunsen-Denkmünze**
15:20 - 15:40	D. Egorova		A. Kushnarenko	B. Voß	B. Finkler	E. Bucher	AWARD LECTURE **Nernst-Haber-Bodenstein-Prize**
15:40 - 16:00	D. Ehmer		K. Dulitz	E. Redel	C. Weinert	S. Stämmler	
	AUDIMAX						
16:00 - 17:00	**Poster Awards and Closing Ceremony** *Chair: M. Peuckert*						
18:00	**ZKM Guided Tour**						
19:00	**Conference Dinner at ZKM** (see page 39)						

OPENING LECTURE

Thursday, May 9, 2013

18:00 – 18:45 **Comparing molecular photofragmentation dynamics in the gas and liquid phases**
Mike Ashfold (University of Bristol/UK)

PLENARY LECTURES

Friday, May 10, 2013

8:30 – 9:15 **Theoretical spectroscopy from molecular dynamics**
Dominik Marx (Ruhr University Bochum/D)

13:30 – 14:15 **Multidimensional spectroscopy of photophysics and photochemistry**
Tobias Brixner (University of Würzburg/D)

Saturday, May 11, 2013

8:30 – 9:15 **Insights into transition metal catalysis from a combination of spectroscopy and quantum chemistry**
Frank Neese (Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D)

13:30 – 14:15 **Interfacial charge transfer dynamics and femtochemistry of molecular adsorbates**
Martin Wolf (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D)

FULL LECTURES

Friday, May 10, 2013

9:20 – 10:00 **IR and UV spectra of cold, biomolecular ions – A challenge for theory**
Thomas Rizzo (École Polytechnique Fédérale de Lausanne/CH)

9:20 – 10:00 **Ionic liquid/metal electrode interfaces: Capacitive processes on different time scales and influence of temperature on interfacial dynamics**
Bernhard Roling (University of Marburg/D)

11:00 – 11:40 **Modeling environment effects on spectroscopies through QM/classical models**
Benedetta Mennucci (University of Pisa/I)

11:00 – 11:40 **Surface sensitive non-linear laser spectroscopy for environmental chemistry research**
Gernot Friedrichs (University of Kiel/D)

14:20 – 15:00 **The THz dance of water with bio-molecules**
Martina Havenith (Ruhr University Bochum/D)

15:00 – 15:40 **From the elementary chemical step to detailed and reduced mechanisms. Kinetics of partially oxidized intermediates**
Thomas Zeuch (University of Göttingen/D)

16:00 – 16:40 **Twenty years of battle with the NO_3 molecule: Some things that I have learned**
John Stanton (University of Texas at Austin/USA)

16:00 – 16:40 **Ultrathin magnetic films: The power of electrochemistry**
Philippe Allongue (CNRS, Palaiseau/F)

Saturday, May 11, 2013

9:20 – 10:00 **Evolution of Kondo resonance from a single impurity molecule to the two-dimensional lattice**
Maki Kawai (University of Tokyo/J)

9:20 – 10:00 **Electrochemistry of metal surfaces under nanoscopic electrolyte layers**
Michael Rohwerder (Max-Planck-Institut für Eisenforschung, Düsseldorf/D)

10:40 – 11:20 **Rotational spectroscopy meets theory**
Cristina Puzzarini (University of Bologna/I)

10:40 – 11:20 **Theoretical studies on the electrode/electrolyte interface**
Timo Jacob (University of Ulm/D)

14:20 – 15:00 **Ultrafast soft X-ray photoelectron spectroscopy at liquid water microjets**
Bernd Abel (University of Leipzig/D)

Thursday, May 9, 2013

	AUDIMAX
	Chair: M. Peuckert
16:30 – 18:00	OPENING CEREMONY Award Ceremony: Award of the Nernst-Haber- Bodenstein-Prize Award of the Bunsen-Denkmünze
18:00 – 18:45	Opening Lecture Comparing molecular photofragmentation dynamics in the gas and liquid phases M. Ashfold, University of Bristol/UK
19:30 – 22:00	Welcome Reception Festsaal Studentenwerk KIT

Friday, May 10, 2013

AUDIMAX

Chair: M. Peuckert

8:30 — **PLENARY LECTURE:**
Theoretical spectroscopy from molecular dynamics
D. Marx, Ruhr University Bochum/D

	AUDIMAX	HÖRSAAL I
	Theory meets Spectroscopy (main topic)	**Interfaces**
	Chair: M. Kappes	*Chair: Y. Joseph*
9:20	**FULL LECTURE** **IR and UV spectra of cold, biomolecular ions – A challenge for theory** T. Rizzo, École Polytechnique Fédérale de Lausanne/CH	**Observation of a transient Stark effect for the indoline dye D149 on electrodeposited ZnO and sintered ZrO_2 and TiO_2 thin films** T. Lenzer, K. Oum, P.W. Lohse, O. Flender, J.R. Klein, University of Siegen/D; M. Scholz, MPI für biophysikalische Chemie, Göttingen/D; J. Du, T. Oekermann, University of Hanover/D
9:40		**Ultraschnelle Relaxationsdynamik von SiO_2 Nanopartikeln nach Anregung im Vakuum-UV Bereich** C. Raschpichler, I. Halfpap, H. Bahro, A. Dorssers, V. Mondes, B. Langer, J. Plenge, E. Rühl, Freie University of Berlin/D; A. Sarfraz, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D; R. Posner, K. Lill, Henkel AG & Co KGaA, Düsseldorf/D; A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D
10:00	**How cations change peptide structure – Insights from theoretical and experimental infrared spectroscopy** C. Baldauf, K. Pagel, S. Warnke, G. von Helden, Fritz-Haber-Institut der MPG, Berlin/D; B. Koksch, Freie Universität Berlin/D; V. Blum, M. Scheffler, Fritz-Haber-Institut der MPG, Berlin/D	**Zirconium oxide based conversion layers on aluminum alloys: Role of intermetallics** A. Sarfraz, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D; R. Posner, K. Lill, Henkel AG & Co KGaA, Düsseldorf/D; A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D
10:20	**Excited state proton transfer reactions in isolated hydroxy-chromones investigated by different IR/UV techniques** A. Stamm, M. Weiler, A. Brächer, K. Schwing, M. Gerhards, TU Kaiserslautern/D	**Critical contact angles on vertical and inclined surfaces: An experimental investigation** M. Schmitt, F. Heib, Saarland University, Saarbrücken/D
10:40	COFFEE BREAK	
	Chair: J. Sauer	*Chair: J.P. Hofmann*
11:00	**FULL LECTURE** **Modeling environment effects on spectroscopies through QM/classical models** B. Mennucci, University of Pisa/I	**FULL LECTURE** **Surface sensitive non-linear laser spectroscopy for environmental chemistry research** G. Friedrichs, University of Kiel/D
11:20		
11:40	**Excited state solvation dynamics of a Reichardt type dye: Water reorientation, chromophore and hydrogen bonding** C. Allolio, Universität Halle-Wittenberg, Halle (Saale)/D; M. Sajadi, N.P. Ernsting, Humboldt-Universität zu Berlin/D; D. Sebastiani, Universität Halle-Wittenberg, Halle (Saale)/D	**Spectroscopic studies and electronic properties of the PTMTC open-shell organic molecules** V. Mugnaini, M. Oliveros, M. Gonidec, I. Alcon, J. Veciana, ICMAB-CSIC, Barcelona/E; R. Ovsyannikov, A. Vollmer, HZB-Bessy II, Berlin/D; A. Calzolari, CNR-Nano, Modena/I; C. Cepek, S. Bhardwaj, M. Kumar, M. Pedio, CNR-IOM, Trieste/I
12:00	**A quantum chemically based model describing enthalpies and free energies of ~300 hydrogen-bond complexes measured by FTIR spectrometry** A. Klamt, J. Reinisch, F. Eckert, COSMOlogic GmbH & Co KG, Leverkusen/D; J. Graton, J.Y. Le Questel, Université de Nantes/F	***In situ* confocal Raman spectroscopy of the crystallization of polypropylene in interface near regions** S. Waschke, C. Kunze, University of Paderborn/D; M. to Baben, J.M. Schneider, RWTH Aachen/D
12:20	LUNCH BREAK	

AUDIMAX

Chair: M. Quack

13:30 – 14:15 — **PLENARY LECTURE:**
Multidimensional spectroscopy of photophysics and photochemistry
T. Brixner, University of Würzburg/D

Friday, May 10, 2013

AUDIMAX

Chair: M. Peuckert

PLENARY LECTURE:
Theoretical spectroscopy from molecular dynamics
D. Marx, Ruhr University Bochum/D — 8:30

	CRIEGEE	HÖRSAAL II
	Industrial Symposium	**Gaseous State**
	Chair: M. Wilhelm	*Chair: M. Olzmann*
9:20	**Detection of explosives by x-ray transmission and other technologies** P. Zänker, Smiths Heimann GmbH, Wiesbaden/D	**Two color enhanced IR spectroscopy of oligonucelar transition metal complexes** M. Gaffga, F. Menges, Y. Nosenko, C. Riehn, G. Niedner-Schatteburg, TU Kaiserslautern/D
9:40		**The formation of fragment ions (H^+, H_3^+, CH_3^+) from ethane in intense femtosecond laser fields – From understanding to control** N. Schirmel, N. Reusch, P. Horsch, K.-M. Weitzel, University of Marburg/D
10:00	**Science behind consumer products: Physics, chemistry and modeling of diapers and superabsorbers** M. Schmidt, Procter & Gamble Service GmbH, Schwalbach am Taunus/D	**Photoionization and photodissociation of halogenated sulfur compounds** B. Kieling, L. Fechner, B. Langer, F. Gerke, R. Flesch, E. Rühl, Freie Universität Berlin/D
10:20		**The photodissociation dynamics of the ethyl radical, C_2H_5, investigated by velocity map imaging** J. Giegerich, M. Steinbauer, K.H. Fischer, I. Fischer, University of Würzburg/D
10:40	COFFEE BREAK	
	Chair: M. Wilhelm	*Chair: J.-U. Grabow*
11:00	**Switchable ultrahydrophobic polymer surfaces – Synthesis, characterization and application** T. Hofe, PSS Polymer Standards Service GmbH, Mainz/D; A. Rollberg, Leibniz Institute of Polymer Research Dresden/D; K. Oleschko, PSS Polymer Standards Service GmbH, Mainz/D; M. Stamm, P. Uhlmann, Leibniz Institute of Polymer Research Dresden/D; T. Beskers, PSS Polymer Standards Service GmbH, Mainz/D; M. Wilhelm, Karlsruhe Institute of Technology/D	**Molecular dynamics and non-adiabatic effects probed via strong-field ionization of state- and isomer-selected molecules fixed in space** S. Trippel, T. Mullins, N. Müller, J. Kienitz, K. Dlugolecki, J. Küpper, DESY, Hamburg/D
11:20		**Low temperature CO oxidation catalyzed by free palladium clusters: Similarities and differences to Pd surfaces and supported particles** S.M. Lang, I. Fleischer, T.M. Bernhardt, University of Ulm/D
11:40	**Time domain NMR studies of industrially relevant processes in polymeric materials** N. Nestle, F. Quero, P. Martin, E. Wassner, BASF SE, Ludwigshafen/D; H. Herold, E. Hardy, Karlsruher Institut für Technologie (KIT)/D	**One and two colour IRMPD-spectra of cold tetranuclear cobalt cluster complexes with carbonyl and bis(diphenylphosphino)amino ligands** J.R. Meyer, M. Gaffga, T. Kolling, J. Mohrbach, G. Niedner-Schatteburg, TU Kaiserslautern/D
12:00	**Flow-induced crystallization in polyolefins: A study using non-linear rheology** I. Vittorias, Basell Polyolefine GmbH, Frankfurt/D	**On the structure of 55 atom transition metal clusters and their relation to the bulk** D. Schooss, T. Rapps, E. Waldt, R. Ahlrichs, M.M. Kappes, Karlsruher Institut für Technologie/D
12:20	LUNCH BREAK	

AUDIMAX

Chair: M. Quack

PLENARY LECTURE:
Multidimensional spectroscopy of photophysics and photochemistry
T. Brixner, University of Würzburg/D — 13:30 – 14:15

Friday, May 10, 2013

	AUDIMAX	
	Chair: M. Peuckert	
8:30	**PLENARY LECTURE:** **Theoretical spectroscopy from molecular dynamics** D. Marx, Ruhr University Bochum/D	
	AOC 101	**HÖRSAAL III**
	Biophysical Chemistry	**Joint Session Solid State / Electrochemical Interfaces**
	Chair: U. Nienhaus	*Chair: R. Schuster*
9:20	**Macromolecular crowding stabilizes the functional, non-toxic state of IAPP by suppressing its fibrillation** J. Seeliger, A. Werkmüller, R. Winter, TU Dortmund/D	**FULL LECTURE** **Ionic liquid/metal electrode interfaces: Capacitive processes on different time scales and influence of temperature on interfacial dynamics** M. Drüschler, B. Roling, University of Marburg/D; N. Borisenko, F. Endres, TU Clausthal/D; R. Atkin, University of Newcastle, Callaghan/AUS
9:40	**Membrane interaction and curvature generation by the coat protein complex I GTPase Arf1p** A. Meister, S. Daum, K. Bacia, Universität Halle-Wittenberg, Halle (Saale)/D	
10:00	**Interactions of short cationic peptides with bilayer membranes and monolayers** A. Hädicke, C. Schwieger, A. Blume, University of Halle-Wittenberg, Halle (Saale)/D	**"Soggy sand" lithium battery electrolytes: Heterogeneous doping for enhanced Li^+ conductivity** J. Popovic, C. Pfaffenhuber, J. Maier, Max Planck Institute for Solid State Research, Stuttgart/D
10:20	**Pressure perturbation of membrane association and intervesicle transfer of lipidated Ras proteins** S. Kapoor, A. Werkmüller, TU Dortmund/D; R.S. Goody, H. Waldmann, Max Planck Institute of Molecular Physiology, Dortmund/D; R. Winter, TU Dortmund/D	**Extremely slow Li exchange processes in diamagnetic Li_2ZrO_3 followed by ^6Li 2D EXSY NMR** P. Bottke, M. Wilkening, TU Graz/A
10:40	COFFEE BREAK	
	Chair: G. Jung	*Chair: B. Roling*
11:00	**Mechanism of multivalent carbohydrate-protein interactions studied by EPR spectroscopy** M. Drescher, Universität Konstanz/D	**Structure and dynamics of the tetragonal LGPS superionic conductor Li_7GePS_8** A. Kuhn, B.V. Lotsch, Max-Planck-Institut für Festkörperforschung, Stuttgart/D
11:20	**UV/Vis and FT-IR spectroscopy reveal how flavin acts as a red light sensor in a cryptochrome blue light receptor** M. Spexard, S. Kakorin, T. Kottke, Universität Bielefeld/D; B. Beel, K. Prager, M. Mittag, Universität Jena/D	**Defect chemistry-based optimization of oxygen deficient nano anatase anodes for lithium ion batteries** D. Samuelis, J.-Y. Shin, J. Maier, Max Planck Institute for Solid State Research, Stuttgart/D
11:40	**Light makes it work. Studies on the molecular reaction dynamics of the enzyme NADPH: Protochlorophyllide-oxidoreductase at ultrafast time scale** A. Garrone, S. Fey, University of Jena/D; J. Schäfer, Institute of Photonic Technology Jena e.V./D; G. Hermann, University of Jena/D; B. Dietzek, Institute of Photonic Technology Jena e.V./D	**Nanoporous n-type silicon as anode for Li-ion batteries** N. Ohmer, Max Planck Institute for Solid State Research, Stuttgart/D; S. Klingbeil, University of Stuttgart/D; M. Reuter, Steinbeis Center Photovoltaics, Stuttgart/D; D. Samuelis, J. Maier, Max Planck Institute for Solid State Research, Stuttgart/D; J.H. Werner, University of Stuttgart and Steinbeis Center Photovoltaics, Stuttgart/D
12:00	**Wavepacket splitting and two-component deactivation in excited isoRhodopsin** O. Weingart, Universität Düsseldorf/D; E. Poli, University of Liverpool/UK; M. Garavelli, Ecole Normale Supérieure de Lyon/F; D. Polli, D. Brida, C. Manzoni, G. Cerullo, Politecnico di Milano/I; K.M. Spillane, P. Kukura, University of Oxford/UK; R.A. Mathies, University of California at Berkeley/USA	**Preparation and characterization of phospho-olivines as cathode materials for Li-ion batteries** M. Kaus, I. Issac, R. Heinzmann, S. Mangold, V.S.K. Chakravadhanula, H. Hahn, S. Indris, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D
12:20	LUNCH BREAK	
	AUDIMAX	
	Chair: M. Quack	
13:30 – 14:15	**PLENARY LECTURE:** **Multidimensional spectroscopy of photophysics and photochemistry** T. Brixner, University of Würzburg/D	

Friday, May 10, 2013

	AUDIMAX	
	Chair: M. Peuckert	
	PLENARY LECTURE: **Theoretical spectroscopy from molecular dynamics** D. Marx, Ruhr University Bochum/D	8:30
	NEUER CHEMIEHÖRSAAL	
	Physical-Chemical Methods	
	Chair: E. Goos	
	Low-pressure effective fluorescence lifetimes of single- and two-ring aromatics and their implication for model development T. Benzler, S. Faust, T. Dreier, C. Schulz, Universität Duisburg-Essen, Duisburg/D	9:20
	Near-field imaging and nano-fourier-transform infrared spectroscopy using broadband synchrotron radiation P. Patoka, Freie Universität Berlin/D; P. Hermann, A. Hoehl, Physikalisch-Technische Bundesanstalt, Berlin/D; E. Rühl, Freie Universität Berlin/D; G. Ulm, Physikalisch-Technische Bundesanstalt, Berlin/D	9:40
	Cavity-enhanced resonant photoacoustic and Raman spectroscopy for trace gas analysis and high-resolution spectroscopy M. Hippler, University of Sheffield/UK	10:00
	Electronically enhanced 2D-IR spectroscopy: Chemical exchange beyond the vibrational lifetime and sub-ensemble selective photochemistry L.J.G.W. van Wilderen, A.T. Messmer, J. Bredenbeck, Universität Frankfurt/D	10:20
	COFFEE BREAK	10:40
	Chair: J. Bredenbeck	
	FT-IR spectroscopy in ultrahigh vacuum: Surface science approach for understanding reactions on catalytic oxide powders X. Stammer, Bruker Optik GmbH, Ettlingen/D; M. Buchholz, S. Heißler, Ch. Wöll, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D	11:00
	Monitoring gas sensors at work: *Operando* Raman-FTIR study of ethanol detection by indium oxide S. Sänze, A. Gurlo, C. Hess, TU Darmstadt/D	11:20
	A millisecond time-resolved infrared-spectroscopy – Mechanistic study on the dehydrogenation of formic acid E. Barsch, D. Mellmann, Leibniz-Institut für Katalyse e.V., Rostock/D; M. Bauer, TU Kaiserslautern/D; H. Junge, Leibniz-Institut für Katalyse e.V., Rostock/D; R. Ludwig, Universität Rostock/D	11:40
	The relation between interfacial charge transport and performance of oxidation catalysts studied with *in situ* microwave techniques M. Eichelbaum, C. Heine, A. Trunschke, R. Schlögl, Fritz-Haber-Institut der MPG, Berlin/D	12:00
	LUNCH BREAK	12:20
	AUDIMAX	
	Chair: M. Quack	
	PLENARY LECTURE: **Multidimensional spectroscopy of photophysics and photochemistry** T. Brixner, University of Würzburg/D	13:30 – 14:15

Friday, May 10, 2013

	AUDIMAX	HÖRSAAL I
	Theory meets Spectroscopy (main topic)	**Interfaces**
	Chair: M. Quack	*Chair: K. Al-Shamery*
14:20	**Anharmonicity in hydrogen bonded clusters: Experimental benchmarks for OH stretching overtones and librations** F. Kollipost, K. Papendorf, Universität Göttingen/D; R. Wugt Larsen, TU of Denmark, Lyngby/DK; M.A. Suhm, Universität Göttingen/D	**Polymer films at the air/water interface studied with infrared reflection absorption spectroscopy (IRRAS)** A. Kerth, Universität Halle-Wittenberg, Halle (Saale)/D; G. Brezesinski, Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam/D; A. Blume, Universität Halle-Wittenberg, Halle (Saale)/D
14:40	**Vibronic coupling and quenching of excitonic splittings in H-bonded molecular dimers** H. Köppel, S. Kopec, Universität Heidelberg/D; P. Ottiger, S. Leutwyler, Universität Bern/CH	**Imidazolium-based ionic liquids interacting with ordered cerium dioxide surfaces: A synchrotron-radiation photoelectron spectroscopy study** M. Laurin, Y. Lykhach, S. Schernich, N. Taccardi, V. Wagner, P. Wasserscheid, H.-P. Steinrück, J. Libuda, FAU Erlangen-Nürnberg, Erlangen/D; N. Tsud, T. Skála, V. Matolín, Charles University, Prague/CZ; K. Prince, Sincrotrone Trieste/I
15:00	**Vibrational spectroscopy of the atmospherically relevant clusters $NO_3^-(HNO_3)_m(H_2O)_n$** N. Heine, Fritz-Haber-Institut der MPG, Berlin/D; T. Yacovitch, University of California, Berkeley/USA; C. Brieger, T. Wende, Fritz-Haber-Institut der MPG, Berlin/D; C. Hock, University of California, Berkeley/USA; K. Asmis, Fritz-Haber-Institut der MPG, Berlin/D; D. Newmark, University of California, Berkeley/USA	**Untersuchung der molekularen Adhäsion von Phosphonsäuren auf Aluminiumoxid-Oberflächen durch AFM basierte Einzelmolekülkraftspektroskopie** B. Ozkaya, B. Mosebach, G. Grundmeier, Universität Paderborn/D
15:20	**The electronic structure and spin density distribution in biomimetic mixed-valence complexes** M. Stein, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; T.B. Rauchfuss, University of Illinois, Urbana/USA	**The wetting properties of graphene in the light of molecular dynamics simulations** F. Leroy, F. Taherian Tabasi, V. Marcon, N.F.A. van der Vegt, TU Darmstadt/D
15:40	COFFEE BREAK	
	Theory meets Spectroscopy (main topic)	**Interfaces**
	Chair: W. Klopper	*Chair: C. Wöll*
16:00	**FULL LECTURE** **Twenty years of battle with the NO_3 molecule: Some things I have learned** J.F. Stanton, University of Texas at Austin/USA	**Bottom-up assembly of tobacco mosaic virus-derived nucleoprotein tubes on defined patterns on silica- and polymer-based substrates** C. Azucena, Karlsruhe Institute of Technology/D; F.J. Eber, University of Stuttgart/D; V. Trouillet, M. Hirtz, S. Heißler, M. Franzreb, H. Fuchs, Karlsruhe Institute of Technology/D; C. Wege, University of Stuttgart/D; H. Gliemann, Karlsruhe Institute of Technology/D
16:20		**Intrinsic switching thermodynamics and kinetics of ultrathin thermoresponsive polymer brushes in halide solutions** C. Amiri Naini, M. Thomas, S. Franzka, S. Frost, M. Ulbricht, N. Hartmann, Universität Duisburg-Essen, Essen/D
16:40	**High-resolution spectroscopy of carbon clusters harboring heavy elements** S. Thorwirth, Universität zu Köln/D	**Photothermal laser processing of titania nanoparticle films** L. Schade, S. Franzka, Universität Duisburg-Essen, Essen/D; S. Hardt, H. Wiggers, Universität Duisburg-Essen, Duisburg/D; N. Hartmann, Universität Duisburg-Essen, Essen/D
17:00	**The last globally stable extended alkane** N.O.B. Lüttschwager, T.N. Wassermann, R. Mata, M.A. Suhm, Universität Göttingen/D	**The role of surface energy on the formation of high spatial frequency laser-induced periodic surface structures** O. Armbruster, M. Lovric, W. Kautek, Universität Wien/A
17:20	**The interplay of electronic and vibrational structure calculations needed for an accurate simulation of infrared spectra** G. Rauhut, University of Stuttgart/D	**Mechanistic study of the pulse laser induced particle separation from polymer surfaces** S. Arif, O. Armbruster, W. Kautek, Universität Wien/A
17:40	**The chemical sensitivity of X-ray spectroscopy: High energy resolution XANES versus valence-to-core X-ray emission spectroscopy** A. Atkins, C. Jacob, Karlsruher Institut für Technologie/D; M. Bauer, TU Kaiserslautern/D	**Highly improved stability of naked gold nanoparticles by *in situ* coating with mono and multivalent thiol PEG ligands** B. Stein, Freie Universität Berlin/D; D. Zopes, S. Mathur, Universität zu Köln/D; C. Graf, Freie Universität Berlin/D
18:00 – 22:00	POSTER SESSION	

Friday, May 10, 2013

	CRIEGEE	HÖRSAAL II
	Industrial Symposium	**Gaseous State**
	Chair: O. Deutschmann	*Chair: A. Fielicke*
14:20	**High throughput experimentation: Tackling future energy challenges with highly efficient R&D tools** T. Mäurer, hte AG, Heidelberg/D	**A comparative theoretical study of the kinetics and dynamics of the reaction of H atoms with ground-state and excited O_2** P. Szabó, University of Pannonia, Veszprém/H; G. Lendvay, Institute for Materials and Environmental Chemistry, Budapest/H
14:40		**Mass spectrometry in flames: Combustion chemistry of iso-pentanol as next-generation biofuel** A. Lucassen, J. Warkentin, N. Hansen, Sandia National Laboratories, Livermore/USA; S.W. Park, M. Sarathy, King Abdullah University of Science and Technology, Thuwal/SAR
15:00	**40 Jahre Autoabgaskatalyse-Forschung: Wie die Katalysator-Entwicklung heute von physikalisch-chemischem Grundlagenwissen profitiert** M. Votsmeier, Umicore AG & Co. KG, Hanau/D	**FULL LECTURE** **From the elementary chemical step to detailed and reduced mechanisms. Kinetics of partially oxidized intermediates** T. Zeuch, University of Göttingen/D
15:20	**Automotive exhaust gas sensing – Current trends** P.A. Neff, Robert Bosch GmbH, Stuttgart/D	
15:40	COFFEE BREAK	
	Industrial Symposium	**Solid State**
	Chair: M. Peuckert	*Chair: D. Samuelis*
16:00	**Simulation of crystallization processes in the food industry** H.J. Limbach, Nestlé Research Center, Lausanne/CH; K. Koschke, D. Donadio, K. Kremer, MPI Polymer Research, Mainz/D	**Activation volume tensor for oxygen vacancy migration in strained CeO_2 electrolytes** J. Hinterberg, T. Zacherle, A.H.H. Ramadan, R.A. De Souza, RWTH Aachen University/D
16:20		**Analysis of strain states in YSZ/rare earth oxide multilayers and their effect on interfacial ionic conductivity and diffusion** J. Keppner, C. Korte, J. Schubert, W. Zander, M. Ziegner, Forschungszentrum Jülich GmbH/D; D. Hesse, Max Planck Institut für Mikrostrukturphysik, Halle/D
16:40	**Filler dispersion in elastomers: Transmission electron microscopy and space statistics** J. Lacayo, Continental Reifen Deutschland GmbH, Hannover/D	**Comparative analysis of oxygen mobility in $(La,Sr)(Co,Fe)O_{3-\delta}$ and $(Ba,Sr)(Co,Fe)O_{3-\delta}$ perovskites based on *ab initio* modeling** R. Merkle, Max Planck Institute for Solid State Research, Stuttgart/D; Y.A. Mastrikov, Institute for Solid State Physics, Riga/LV; E.A. Kotomin, Max Planck Institute for Solid State Research, Stuttgart/D; M.M. Kuklja, University of Maryland/USA; J. Maier, Max Planck Institute for Solid State Research, Stuttgart/D
17:00		**Conductivity of pure and cation doped $Ca_{12}Al_{14}O_{33-\delta}$** R. Dolle, H.-D. Wiemhöfer, Universität Münster/D; J.-P. Eufinger, D.-K. Lee, J. Janek, Universität Gießen/D; H. Krause, S. Ebbinghaus, Universität Halle-Wittenberg, Halle (Saale)/D
17:20	**Analysis of polymer coatings and laminates by automated FTIR microscopy** M. Luft, M. Boese, Bruker Optik GmbH, Ettlingen/D	**Electrical conductivity of CeO_2: Size matters** G. Gregori, M.C. Göbel, M. Shirpour, R. Merkle, J. Maier, Max-Planck-Institut für Festkörperforschung, Stuttgart/D
17:40		**A high-temperature Mössbauer study of iron-doped Ruddlesden-Popper phases $La_{n+1}Ni_nO_{3n+1}$** P. Gaczynski, TU Braunschweig/D; T. Klande, A. Feldhoff, Leibniz Universität Hannover/D; K.-D. Becker, TU Braunschweig/D
18:00 – 22:00	POSTER SESSION	

Friday, May 10, 2013

	AOC 101	HÖRSAAL III
	Biophysical Chemistry	**Electrochemical Interfaces**
	Chair: T. Kottke	*Chair: A. Kuhn*
14:20	**FULL LECTURE** **The THz dance of water with bio-molecules** M. Havenith, Ruhr University Bochum/D	**Li-rich spinel $Li_{1+x}FeTiO_4$ as cathode materials for Li-ion batteries** R. Chen, R. Heinzmann, R. Witte, S. Lebedkin, H. Hahn, S. Indris, Karlsruher Institut für Technologie/D
14:40		**Modelling mass and charge transport in different types of electrolytes and impact on Li-ion cell performance** M. Mutke, H.-D. Wiemhöfer, Universität Münster/D
15:00	**Non-linear optical imaging – A tool to discriminate healthy skin against non-melanoma skin cancers?** S. Heuke, N. Vogler, T. Meyer, D. Akimov, Institut für Photonische Technologien Jena e.V./D; K. Franziska, H.-J. Röwert-Huber, J. Lademann, Universitätsklinikum Berlin - Charité/D; J. Popp, Institut für Photonische Technologien Jena e.V./D	**Modeling crystallization in lithium-oxygen batteries** B. Horstmann, Deutsches Zentrum für Luft- und Raumfahrt, Stuttgart/D and Helmholtz-Institut Ulm/D
15:20	**Isotope labelled infrared spectroscopy and theoretical investigations of adenosine 5'-di- and triphosphate anions in a penning trap** F. Schinle, P.E. Crider, O. Hampe, M.M. Kappes, Karlsruher Institut für Technologie/D	**Investigations of lithium dendrite growth** S.L. Koch, E. Paillard, M. Winter, S. Passerini, University of Münster/D
15:40	COFFEE BREAK	
	Biophysical Chemistry	**Electrochemical Interfaces**
	Chair: B. Luy	*Chair: R. Schuster*
16:00	**Skin from the chemical perspective – Raman micro-spectroscopy for disease characterization and therapy surveillance** M. Mischo, Ruhr-Universität Bochum/D; L. von Kobyletzki, Lund University, Malmö/S; L. von Kobyletzki, Karlstad University/S; S. Baldus, D. Schmidt, A. Potthoff, E. Bründermann, N.H. Brockmeyer, P. Awakowicz, M. Havenith, Ruhr-Universität Bochum/D	**FULL LECTURE** **Ultrathin magnetic films: The power of electrochemistry** P. Allongue, F. Maroun, N. Tournerie, A. Engelhardt, R. Novak, CNRS, Palaiseau/F
16:20	**Understanding biomolecular hydration-shell dynamics at the molecular level** A. Fogarty, Ecole Normale Supérieure, Paris/F; F. Sterpone, IBPC, Paris/F; J.T. Hynes, University of Colorado, Boulder/USA; D. Laage, Ecole Normale Supérieure, Paris/F	
16:40	**A thermodynamic view on protein affinities to aqueous-solid interfaces** J. Koo, C. Czeslik, TU Dortmund/D	**Porous nanophase materials with electrochemically tunable properties** E. Steyskal, S. Topolovec, S. Landgraf, TU Graz/A; H. Krenn, Universität Graz/A; R. Würschum, TU Graz/A
17:00	**Small affinity molecules for large recognitions** A.M. Kreuziger, C. Schmidtke, J. Ostermann, H. Weller, Universität Hamburg/D	***In situ* spectroelectrochemical investigation of semiconductor electrodeposition in ionic liquids** A. Lahiri, O. Höfft, S. Zein El Abedin, F. Endres, TU Clausthal/D
17:20	**Conjugation of iron oxide nanoparticles to a cancer-specific antibody for a highly sensitive MRI cancer detection and characterisation** S.C. Salmen, University of Hamburg/D; M. Heine, A. Schildt, N. Raabe, U. Schumacher, G. Adam, University Medical Center Hamburg-Eppendorf/D; H. Weller, University of Hamburg/D	**Evidence for SERRS-enhancement in the spectra of ruthenium-dye metal nanoparticle conjugates** F. Theil, L. Zedler, A. März, University of Jena/D; W. Xie, University of Osnabrück/D; A. Csaki, W. Fritzsche, D. Cialla, Institut für Photonische Technologien Jena e.V./D; M. Schmitt, University of Jena/D; J. Popp, B. Dietzek, Institut für Photonische Technologien Jena e.V./D
17:40	**When stem cells roll: A microfluidic analysis of the catch bond mediated interaction between CD44 and hyaluronic acid** M. Hanke, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D; I. Taubert, C. Christophis, N. Baran, P. Wuchter, A. Ho, Universitätsklinikum Heidelberg/D; A. Rosenhahn, Ruhr-Universität Bochum/D	**Shear elasticity in liquids: A quartz crystal microbalance study** W.E. Gomes, M.A. Tenan, E.R.R. do Nascimento, C.A. Bertran, Universidade Estadual de Campinas/BR; W. Kautek, Universität Wien/A; D.M. Soares, Universidade Estadual de Campinas/BR
18:00 – 22:00	**POSTER SESSION**	

Friday, May 10, 2013

	NEUER CHEMIEHÖRSAAL	
	Physical-Chemical Methods	
	Chair: M. Hippler	
14:20	**Liquid beam ion desorption mass spectrometry for evaluating CASSINI data** F. Stolz, Universität Leipzig/D; R. Reviol, Universität Heidelberg/D; R. Srama, Universität Stuttgart/D; M. Trieloff, F. Postberg, Universität Heidelberg/D; B. Abel, Leibniz Institut für Oberflächen-modifizierung (IOM)/D	
14:40	**Laser photofragmentation and ultrafast time-resolved dynamics of mass-selected metal-ligand ionic species** C. Riehn, Y. Nosenko, D. Imanbaew, S. Kruppa, TU Kaiserslautern/D	
15:00	**Band structure investigations of organic single crystals using a novel multidimensional electron spectrometer: ARTOF 10k** A. Vollmer, R. Ovsyannikov, M. Gorgoi, M. Oehzelt, S. Krause, A. Föhlisch, Helmholtz Zentrum Berlin für Materialien und Energie GmbH/D; N. Martensson, S. Svensson, A. Lindblad, Uppsala University/S; T. Schmeiler, J. Pflaum, Universität Würzburg/D; N. Koch, Humboldt Universität zu Berlin/D	
15:20	**Crosslinked gold nanoparticles on polyethylene: Resistive responses to tensile strain and vapors** N. Olichwer, E.W. Leib, A.H. Halfar, A. Petrov, T. Vossmeyer, Universität Hamburg/D	
	COFFEE BREAK	15:40
	Physical-Chemical Methods	
	Chair: A. Köhn	
16:00	**Kinetic Monte Carlo simulations of heterogeneously catalyzed gas-phase reactions** F.M. Kuhn, L. Kunz, O. Deutschmann, Karlsruher Institut für Technologie/D	
16:20	**First principles simulations of vibrationally resolved photodetachment spectra of select biradicals using MCTDH** M. Nooijen, P. Goel, University of Waterloo/CDN	
16:40	**Accurate photoelectron spectra from first principles: How to find a reliable DFT starting point for G_0W_0** T. Körzdörfer, University of Potsdam/D	
17:00	**Temperature effect of the fluorescence blueshift in [n]cycloparaphenylenes with increasing molecular size** S. Irle, C. Camacho, Nagoya University/J; T. Niehaus, University of Regensburg/D	
17:20	**Electron dynamics of excitation induced interatomic coulombic decay in quantum dots** A. Bande, K. Gokhberg, L.S. Cederbaum, Universität Heidelberg/D	
17:40	**Size dependent vibrational frequency shift of CO^+ ions inside helium clusters** M. Lewerenz, M. Mladenovic, Universite Paris Est, Marne la Vallee Cedex 2/F	
	POSTER SESSION	18:00 – 22:00

Saturday, May 11, 2013

	AUDIMAX	
	Chair: W. Domcke	
8:30	**PLENARY LECTURE:** **Insights into transition metal catalysis from a combination of spectroscopy and quantum chemistry** F. Neese, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D	
	AUDIMAX	HÖRSAAL I
	Theory meets Spectroscopy (main topic)	**Interfaces**
	Chair: W. Domcke	*Chair: A. Turchanin*
9:20	**FULL LECTURE** **Evolution of Kondo resonance from a single impurity molecule to the two-dimensional lattice** M. Kawai, University of Tokyo/J	**Gasdetektion mit komplexen SPR-Sensoren und ellipsometrischem Messprinzip** A. Hertwig, A. Nooke, U. Beck, A. Krause, BAM Bundesanstalt für Materialforschung und -prüfung, Berlin/D; M. Kormunda, J. Pavlik, University Jan Evangelista Purkyne, Usti nad Labem/CZ; H. Krüger, V. Lohse, V. Schröder, BAM Bundesanstalt für Materialforschung und -prüfung, Berlin/D; J. Steinbach, Technische Universität Berlin/D
9:40		**Metallorganische Netzwerke: Chemiresistoren aus dem Baukasten** R. Dittrich, M. Günthel, J. Hübscher, M. Mazik, F. Mertens, Y. Joseph, TU Bergakademie Freiberg/D
10:00	***Ab initio* assignment of NMR spectra using linear- and sublinear-scaling quantum-chemical methods for molecules with 1000 and more atoms** C. Ochsenfeld, University of Munich/D	**Structured surface-anchored metal-organic frameworks: A new class of highly porous material with high potential for biological application** H. Gliemann, M. Hanke, H.K. Arslan, S. Bauer, O. Zybaylo, C. Christophis, A. Rosenhahn, C. Wöll, Karlsruhe Institute of Technology/D
10:20	COFFEE BREAK	
	Chair: M. Schnell	*Chair: W. Kautek*
10:40	**FULL LECTURE** **Rotational spectroscopy meets theory** C. Puzzarini, University of Bologna/I	**C_{58} on Au(111): An STM-based study** N. Bajales, S. Schmaus, T. Miyamachi, W. Wulfhekel, J. Wilhelm, M. Stendel, M. Walz, A. Bagrets, F. Evers, S. Ulas, B. Kern, A. Böttcher, M.M. Kappes, Karlsruher Institut für Technologie/D
11:00		**Surface-assisted organic synthesis: Novel hyperbenzene nanotroughs and coordination polymer chains on Cu(111)** Q.T. Fan, C.C. Wang, Y. Han, J.F. Zhu, University of Science and Technology of China, Hefei/PRC; W. Hieringer, FAU Erlangen-Nürnberg, Erlangen/D; J. Kuttner, G. Hilt, J.M. Gottfried, Universität Marburg/D
11:20	**The hydrogen bonding in vitamin C: A puzzle disentangled** I. Peña, A.M. Daly, C. Cabezas, S. Mata, C. Bermúdez, A. Niño, J.C. López, J.L. Alonso, Universidad de Valladolid/E; J.-U. Grabow, Leibniz-Universität Hannover/D	**Electronic properties of MoV oxide catalysts in the selective oxidation of alkanes: An *in situ* microwave cavity perturbation study** C. Heine, M. Eichelbaum, A. Trunschke, R. Schlögl, Fritz-Haber-Institut der MPG, Berlin/D
11:40	**Internal rotation and nuclear quadrupole splitting measured with broadband microwave spectroscopy** V.A. Shubert, D. Schmitz, T. Betz, M. Schnell, Center for Free Electron Science, Hamburg/D	**Towards atomistic simulations of heterogeneous catalysts employing neural network potentials** N. Artrith, B. Hiller, T. Morawietz, J. Behler, Ruhr-Universität Bochum/D
12:00	**A joint venture in microwave spectroscopy, quantum chemistry, and X-ray diffraction: The conformational space of small odorant molecules** H. Mouhib, W. Stahl, C. Merkens, T. Stadtmüller, U. Englert, RWTH Aachen University/D	**Surface vibrational spectroscopy of multi-unsaturated hydrocarbons on model catalysts** S. Schauermann, W. Ludwig, A. Savara, K.-H. Dostert, C.P. O'Brien, H.-J. Freund, Fritz-Haber-Institut der MPG, Berlin/D
12:20 – 13:30	LUNCH BREAK	

Saturday, May 11, 2013

	AUDIMAX		
	Chair: W. Domcke		
8:30	**PLENARY LECTURE:** **Insights into transition metal catalysis from a combination of spectroscopy and quantum chemistry** F. Neese, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D		8:30
	CRIEGEE	HÖRSAAL II	
	Theory meets Spectroscopy (main topic)	**Solid State**	
	Chair: A. Bande	*Chair: E. Bucher*	
9:20	**Low scaling second-order methods for excited states using pair natural orbitals** B. Helmich, C. Hättig, Ruhr-Universität Bochum/D	**Mixed conducting perovskite-type electrodes in H_2/H_2O and O_2 atmospheres: Current pathways and electrode kinetics** A.K. Opitz, A. Nenning, S. Kogler, G. Walch, J. Fleig, TU Wien/A	9:20
9:40	**An incremental correlation approach to electronic excitation energies in molecular systems** R.A. Mata, Universität Göttingen/D	**Fast fluorine ion conductivity in fluorite-type $Ba_xLa_{1-x}F_{3-x}$ solid solutions prepared by high-energy ball milling** A. Düvel, P. Heitjans, Leibniz Universität Hannover/D	9:40
10:00	**Electron tunneling from electronically excited states of chromophore multianions** M.-O. Winghart, Karlsruher Institut für Technologie/D; J.-P. Yang, Hefei University of Technology/PRC; M. Kühn, A.-N. Unterreiner, T. Wolf, Karlsruher Institut für Technologie/D; P.D. Dau, H.-T. Liu, D.-L. Huang, Brown University, Providence/USA; Y.-R. Miao, C.-G. Ning, Tsinghua University, Beijing/PRC; W. Klopper, Karlsruher Institut für Technologie/D; L.-S. Wang, Brown University, Providence/USA; M.M. Kappes, Karlsruher Institut für Technologie/D	**Bombardment induced transport of Rb^+ through a K^+ conducting glass versus K^+ through a Rb^+ glass** D. Budina, J. Martin, P. Menezes, J. Zakel, M. Schäfer, K.-M. Weitzel, Universität Marburg/D	10:00
10:20	COFFEE BREAK		10:20
	Chair: G. Rauhut	*Chair: G. Gregori*	
10:40	**Analytic hessians and vibrational spectra calculations for RI-CC2 and RI-MP2** D. Friese, C. Hättig, Ruhr-Universität Bochum/D	**Converse piezoelectricity** M. Springborg, Saarland University, Saarbrücken/D; B. Kirtman, University of California, Santa Barbara/USA	10:40
11:00	**Dissecting the interaction energies in ionic liquids by means of low frequency spectroscopy and quantum chemical calculations** K. Fumino, Universität Rostock/D; V. Fossog, Universität des Saarlandes, Saarbrücken/D; K. Wittler, Universität Rostock/D; R. Hempelmann, Universität des Saarlandes, Saarbrücken/D; R. Ludwig, Universität Rostock/D	**Atomic scale insight into the oxidation of Ru(0001) using atomic oxygen** B. Herd, J. Goritzka, H. Over, University of Giessen/D	11:00
11:20	**Computing vibrational spectra from *ab initio* molecular dynamics** M. Thomas, M. Brehm, R. Fligg, P. Vöhringer, B. Kirchner, Universität Bonn/D	**Operando XAS study on Pd_2Ga catalyst for methanol synthesis** H.W. Pereira de Carvalho, Karlsruhe Institute of Technolgy/D; I. Sharafutdinov, TU of Denmark, Lyngby/DK; H. Lichtenberg, Karlsruhe Institute of Technolgy/D; I. Chorkendorff, C. Damsgaard, TU of Denmark, Lyngby/DK; J.D. Grunwaldt, Karlsruhe Institute of Technolgy/D	11:20
11:40	**The ClO dimer: Structures, spectroscopy, formation and thermochemistry** L. Horny, M. Willeke, M. Quack, ETH Zürich/CH	**Triplet exciton dynamics in single-wall carbon nanotubes** F. Späth, D. Stich, H. Kraus, A. Sperlich, V. Dyakonov, T. Hertel, Universität Würzburg/D	11:40
12:00	**Computational dielectric spectroscopy of charged, dipolar systems** O. Steinhauser, M. Haberler, C. Schroeder, Universität Wien/A	**New mixed crystals containing nanoparticles as color conversion materials** T. Otto, M. Müller, P. Mundra, TU Dresden/D; V. Lesnyak, Istituto Italiano di Tecnologia, Genua/I; H.V. Demir, TU Nanyang, Singapur/SGP; N. Gaponik, A. Eychmüller, TU Dresden/D	12:00
12:20 – 13:30	LUNCH BREAK		12:20 – 13:30

Saturday, May 11, 2013

	AUDIMAX	
	Chair: W. Domcke	
8:30	**PLENARY LECTURE:** **Insights into transition metal catalysis from a combination of spectroscopy and quantum chemistry** F. Neese, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D	
	AOC 101	**HÖRSAAL III**
	Soft Matter	**Electrochemical Interfaces**
	Chair: C. Czeslik	*Chair: B. Horstmann*
9:20	**Effect and evolution of nanostructural complexity in sensitive polymer gels** S. Seiffert, Helmholtz-Zentrum Berlin/D	**FULL LECTURE** **Electrochemistry of metal surfaces under nanoscopic electrolyte layers** M. Rohwerder, Max-Planck-Institut für Eisenforschung, Düsseldorf/D
9:40	**New approaches for efficient simulation of complex molecules and aggregates** B. Engels, Universität Würzburg/D	
10:00	**How micelle curvature and charge density determine the structure of mixtures with oppositely charged polyelectrolytes** L. Chiappisi, M. Gradzielski, TU Berlin/D	**Probing interfacial layer thickness and electronic properties of electrochemical interfaces: The example of oxide on zinc** Y. Chen, A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D
10:20	COFFEE BREAK	
	Chair: S. Seiffert	*Chair: C. Roth*
10:40	**Excess entropy scaling of transport properties of polyethylene chains** E. Voyiatzis, M.C. Böhm, F. Müller-Plathe, TU Darmstadt/D	**FULL LECTURE** **Theoretical studies on the electrode/electrolyte interface** T. Jacob, University of Ulm/D
11:00	**Properties of star-shaped polymers tethered to a flat surface investigated by Monte Carlo simulation studies** S. Eisenhaber, G. Zifferer, Universität Wien/A	
11:20	**A novel series of metastable SURMOF-2 and their post synthetic modifications** J. Liu, Z. Wang, H.K. Arslan, P. Weidler, H. Gliemann, S. Bräse, S. Grosjean, C. Wöll, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D; B. Lukose, T. Heine, Jacobs-University Bremen/D; A. Godt, Bielefeld University/D; X. Feng, K. Müllen, Max-Plank-Institut für Polymerforschung, Mainz/D	**Catching intermediates of the oxygen reduction reaction *in situ*: Insights from electrochemical ATIR-IR and DFT** P.U. Biedermann, S. Nayak, A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D
11:40	**Confocal Raman microscopy: True surface and 3D Raman imaging** M. Stadler, U. Schmidt, T. Dieing, O. Hollricher, WITec GmbH, Ulm/D	**NiPt nanoparticles with independently tunable size and composition as electrocatalyst for fuel cell applications** L. Wittern, H. Heller, H. Weller, Universität Hamburg/D
12:00	**Smectic C phases in ionic liquid crystals** N. Kapernaum, C. Müller, S. Klenk, G. Starkulla, S. Laschat, F. Giesselmann, Universität Stuttgart/D	**3D porous graphene-based composites for electrocatalytic applications** H. Natter, A. Marinkas, Saarland University, Saarbrücken/D; V. Peinecke, A. Heinzel, ZBT Duisburg/D
12:20 – 13:30	LUNCH BREAK	

Saturday, May 11, 2013

	AUDIMAX	
	Chair: W. Domcke	
	PLENARY LECTURE: **Insights into transition metal catalysis from a combination of spectroscopy and quantum chemistry** F. Neese, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr/D	8:30
	NEUER CHEMIEHÖRSAAL	
	Hot Topics	
	Chair: M. Quack	
	Tunneling and tunneling switching dynamics in phenol and o-D-phenol: FTIR spectroscopy with synchrotron radiation and theory S. Albert, ETH Zürich/CH; Ph. Lerch, PSI, Villigen/CH; R. Prentner, M. Quack, ETH Zürich/CH	9:20
	High-harmonic spectroscopy of oriented polyatomic molecules P. Kraus, A. Rupenyan, J. Schneider, H.J. Wörner, ETH Zürich/CH	9:40
	PIRATS study of oxygenates on titania P.M. Clawin, Universität Oldenburg/D; C.M. Friend, Harvard University, Cambridge/USA; K. Al-Shamery, Universität Oldenburg/D	10:00
	COFFEE BREAK	10:20
	Chair: R. Schäfer	
	A synchrotron-based micro-X-ray diffraction study on the intergrowth structure of large H-ZSM-5 crystals J.P. Hofmann, Z. Ristanovic, U. Deka, Z. Öztürk, Utrecht University/NL; T. Schülli, European Synchrotron Radiation Facility, Grenoble/F; A.M. Beale, B.M. Weckhuysen, Utrecht University/NL	10:40
	Single-particle photoluminescence microscopy of carbon nanotubes under microfluidic and potentiostatic control N. Rühl, T. Hertel, Universität Würzburg/D	11:00
	Electrically-driven molecular motors: Unidirectional motion and inelastic electron tunneling T. Kudernac, University of Groningen/NL; M. Parschau, Empa, Duebendorf/CH; N. Ruangsupapichat, B. Macia, N. Katsonis, S. Harutyunyan, B.L. Feringa, University of Groningen/NL; K.-H. Ernst, Empa, Duebendorf/CH	11:20
	Carbon nanomembranes and graphene from aromatic molecules P. Angelova, H. Vieker, N.-E. Weber, D. Matei, Universität Bielefeld/D; S. Kurash, U. Kaiser, Universität Ulm/D; K. Müllen, Max Planck Institut für Polymerforschung, Mainz/D; A. Turchanin, A. Gölzhäuser, Universität Bielefeld/D	11:40
	ATR-IR spectroscopic study of H_2O and D_2O in one-dimensional confinement S. Nayak, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D; Sriram, C. Chia-Fu, Academia Sinica, Taipei/TW; A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D	12:00
LUNCH BREAK		12:20 – 13:30

Saturday, May 11, 2013

	AUDIMAX	
	Chair: J. Gauß	
13:30	**PLENARY LECTURE:** **Interfacial charge transfer dynamics and femtochemistry of molecular adsorbates** M. Wolf, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D	
	AUDIMAX	
	Theory meets Spectroscopy (main topic)	
	Chair: J. Gauß	
14:20	**FULL LECTURE** **Ultrafast soft X-ray photoelectron spectroscopy at liquid water microjets** B. Abel, University of Leipzig/D	
14:40		
15:00	**Structures of magnetic lanthanide clusters from far-IR spectroscopy** J. Bowlan, FU Berlin/D; D.J. Harding, Universität Göttingen/D; J. Jalink, A. Kirilyuk, G. Meijer, Radboud University Nijmegen/NL; A. Fielicke, TU Berlin/D	
15:20	**Theoretical speculations on capabilities of two-dimensional electronic photon-echo spectroscopy to resolve coherent molecular dynamics** D. Egorova, Universität zu Kiel/D	
15:40	**Femtosecond two-dimensional infrared spectroscopy of aniline: Experiment and *ab initio* calculations** D. Ehmer, D. Czurlok, J. Lindner, P. Vöhringer, Universität Bonn/D	
	AUDIMAX	
	Chair: M. Peuckert	
16:00 – 17:00	**Poster Awards and Closing Ceremony**	
18:00	**Guided Tour of the ZKM** Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*	
19:00	**Conference Dinner at the ZKM** Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*	

Saturday, May 11, 2013

	AUDIMAX		
	Chair: J. Gauß		
13:30	**PLENARY LECTURE:** **Interfacial charge transfer dynamics and femtochemistry of molecular adsorbates** M. Wolf, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D		13:30
	CRIEGEE	**HÖRSAAL II**	
	Theory meets Spectroscopy (main topic)	**Solid State**	
	Chair: K. Fink	*Chair: M. Springborg*	
14:20	**Photoinduced electron transfer with triplet states of N-phthalimides** F.J. Ifthikar, International University, Islamabad/PK; A. Mansha, GC University, Faisalabad/PK; G. Grampp, A. Kelterer, Graz University of Technology/A	**Li-ion mobility in rutile TiO_2 as anode material for Li-ion batteries studied by ^{7}Li NMR** M. Scheuermann, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D; M. Wohlfahrt-Mehrens, Zentrum für Solarenergie und Wasserstoff Forschung, Ulm/D; N. Hüsing, Universität Salzburg/A; S. Indris, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D	14:20
14:40	**On the treatment of solvent effects for electronically excited molecules using continuum models** B. Lunkenheimer, A. Köhn, Universität Mainz/D	**Selective placement of faceted metal tips on semiconductor nanorods** H. Schlicke, D. Ghosh, L.-K. Fong, University of California Berkeley and Lawrence Berkeley National Laboratory, CA/USA; H.L. Xin, H. Zheng, Lawrence Berkeley National Laboratory, CA/USA; A.P. Alivisatos, University of California Berkeley and Lawrence Berkeley National Laboratory, CA/USA	14:40
15:00	**Controlling photochemistry via remote substitution** T.N.V. Karsili, A.M. Wenge, M.N.R. Ashfold, University of Bristol/UK	**Size, shape and composition control of copper-based nanocrystals** M. Kruszynska, J. Li, B. Kempken, J. Parisi, J. Kolny-Olesiak, Universität Oldenburg/D	15:00
15:20	**Femtosecond investigation of intramolecular energy redistribution driven by different chromophore states** A. Kushnarenko, E. Miloglyadov, M. Quack, G. Seyfang, ETH Zürich/CH	**Aufklärung des Urspungs der engen Partikelgrößenverteilung von hexagonalen $NaSEF_4$ (SE = Sm, Eu, Gd, Tb) Nanopartikeln** B. Voß, M. Haase, Universität Osnabrück/D	15:20
15:40	**Towards cold chemistry with magnetically decelerated hydrogen atoms** K. Dulitz, University of Oxford/UK; M. Motsch, ETH Zürich/CH; N. Vanhaecke, Fritz-Haber-Institut der MPG, Berlin/D; T.P. Softley, University of Oxford/UK	**Photonic & optical tunable nanomaterials** E. Redel, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D	15:40
	AUDIMAX		
	Chair: M. Peuckert		
16:00 – 17:00	**Poster Awards and Closing Ceremony**		16:00 – 17:00
18:00	**Guided Tour of the ZKM** Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*		18:00
19:00	**Conference Dinner at the ZKM** Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*		19:00

Saturday, May 11, 2013

	AUDIMAX	
	Chair: J. Gauß	
13:30	**PLENARY LECTURE:** **Interfacial charge transfer dynamics and femtochemistry of molecular adsorbates** M. Wolf, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D	
	AOC 101	**HÖRSAAL III**
	Liquid State	**Electrochemical Interfaces**
	Chair: W. von Rybinski	*Chair: R. Merkle*
14:20	**Time-resolved photoelectron spectroscopy on liquids: How fast is the evaporation of water?** E. Lugovoy, T. Gladytz, J. Nilsson, Universität Leipzig/D; B. Abel, K.R. Siefermann, Leibniz Institut für Oberflächenmodifizierung/D	**Solar hydrogen evolution by novel metal-free polymeric carbon nitride/chalcopyrite composite photocathodes** F. Yang, M. Pogrzeba, V. Kuznietzov, C. Merschjann, Helmholtz Zentrum Berlin/D; M. Lublow, Leibniz-Institut für Katalyse e.V., Rostock/D; A. Thomas, TU Berlin/D; T. Schedel-Niedrig, Helmholtz Zentrum Berlin/D
14:40	**The THz signature of single ions in aqueous solution** G. Schwaab, F. Böhm, V. Sharma, H. Wirtz, M. Havenith, Ruhr-Universität Bochum/D	**Bombardment induced ion transport (BIIT) through ultra-thin polymer films** S. Schulze, J. Zakel, M. Schäfer, A. Greiner, K.-M. Weitzel, Universität Marburg/D
15:00	**Ion speciation of protic ionic liquids in water: Transfer from contact to solvent-separated ion pairs** P. Stange, K. Fumino, R. Ludwig, Universität Rostock/D	**Oxygen diffusion in single crystal and bicrystal $SrTiO_3$** V. Metlenko, R.A. De Souza, RWTH Aachen University/D
15:20	**Solvent dependent characterization of highly photostable super-photoacids** B. Finkler, C. Spies, G. Jung, Saarland University, Saarbrücken/D	**Surface sensitivity of $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ to SO_2 trace-impurities** E. Bucher, W. Sitte, Montanuniversität Leoben/A; Ch. Gspan, F. Hofer, TU Graz and Graz Center for Electron Microscopy (ZFE)/A
15:40	**Ultrafast electronic relaxation and ground state cooling dynamics of Triphenylverdazyl radicals in acetonitrile** C. Weinert, B. Wezisla, J. Lindner, P. Vöhringer, Universität Bonn/D	**Enhanced oxygen exchange at $(La,Sr)CoO_{3-\delta}$ / $(La,Sr)_2CoO_{4+\delta}$ / O_2 triple phase boundaries** S. Stämmler, R. Merkle, B. Stuhlhofer, G. Logvenov, J. Maier, Max Planck Institute for Solid State Research, Stuttgart/D
	AUDIMAX	
	Chair: M. Peuckert	
16:00 – 17:00	**Poster Awards and Closing Ceremony**	
18:00	**Guided Tour of the ZKM** Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*	
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Saturday, May 11, 2013

	AUDIMAX	
	Chair: J. Gauß	
13:30	**PLENARY LECTURE:** **Interfacial charge transfer dynamics and femtochemistry of molecular adsorbates** M. Wolf, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D	13:30
	NEUER CHEMIEHÖRSAAL	
	Joint Session DFG Funding / DBG Awards	
	Chair: M. Peuckert	
14:20	**Position und Gestaltungsmöglichkeiten der Physikalischen Chemie in der DFG** J. Kowol-Santen, K. Winkler, Deutsche Forschungsgemeinschaft (DFG), Bonn/D	14:20
		14:40
	AWARD LECTURE **Bunsen-Denkmünze**	15:00
		15:20
	AWARD LECTURE **Nernst-Haber-Bodenstein-Prize**	15:40
	AUDIMAX	
	Chair: M. Peuckert	
	Poster Awards and Closing Ceremony	16:00 – 17:00
	Guided Tour of the ZKM Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*	18:00
	Conference Dinner at the ZKM Zentrum für Kunst und Medientechnologie Karlsruhe *(Center for Art and Media Karlsruhe)*	19:00

Theory meets Spectroscopy (main topic)

P 1.01 **The Raman spectrum of water clusters**
K.E. Otto, Z. Xue, P. Zielke, M.A. Suhm, University of Göttingen/D

P 1.02 **Mechanism of protonation induced changes in the photophysical properties of a molecular DNA sensor**
M. Wächtler, M. Bräutigam, University of Jena/D; S. Rau, University of Ulm/D; J. Popp, B. Dietzek, University of Jena/D

P 1.03 **Origin-independent calculation of quadrupole intensities in X-ray spectroscopy**
A.J. Atkins, S. Bernadotte, C.R. Jacob, Karlsruhe Institute of Technology (KIT)/D

P 1.04 **Thermosensitivity of copolymers of *N*-isopropylacrylamide and *N,N*-diethylacrylamide: The influence of monomer sequence and methanol addition**
F. Plamper, C. Hofmann, A. Steinschulte, RWTH Aachen University/D; R. Winter, TU Dortmund/D; S. Hietala, University of Helsinki/FIN; W. Richtering, RWTH Aachen University/D

P 1.05 **Preferential solvation on radical ion pair detected by MARY spectroscopy**
K. Pal, G. Grampp, D.R. Kattnig, S. Landgraf, TU Graz/A

P 1.06 **A quantum-mechanical study of selected molecules: Influence of the reactant and the functional group on their vibrational spectra**
M. Ramirez, F. Flug, C. Nies, M. Springborg, W. Possart, Saarland University, Saarbrücken/D

P 1.07 **Analysis of o-carborane based donor-acceptor-dyes by static and dynamic fluorescence methods**
L. Böhling, J. Kahlert, A. Brockhinke, L. Weber, Universität Bielefeld/D; M.A. Fox, Durham University/UK

P 1.08 **Fullerene ions in outer space and in the laboratory**
D. Strelnikov, B. Kern, P. Weis, A. Böttcher, M.M. Kappes, Karlsruher Institut für Technologie/D

P 1.09 **Analyzing vibrational spectra of polymers with localized modes**
P.T. Panek, C.R. Jacob, Karlsruhe Institute of Technology/D

P 1.10 **Efficient calculation of high-order coupling terms in the many-body expansion of potential energy surfaces**
P. Meier, J. Klepp, G. Rauhut, Universität Stuttgart/D; G. Bellchambers, F.R. Manby, University of Bristol/UK

P 1.11 **Implementation of two-component time-dependent density functional theory and application to phosphorescence lifetimes of OLEDs**
M. Kühn, F. Weigend, Karlsruher Institut für Technologie/D

P 1.12 **Aggregation of 1-indanol: A multiexperimental approach reveals chirality recognition phenomena at the edge of DFT accuracy**
J. Altnöder, J.J. Lee, K.E. Otto, M.A. Suhm, Universität Göttingen/D; A. Bouchet, M. Broquier, A. Zehnacker-Rentien, Université Paris-Sud/F

P 1.13 **Onset of hydrogen bonded collective network of water in 1,4-dioxane**
T.Q. Luong, Ruhr University Bochum/D; P.K. Verma, R.K. Mitra, S.N. Bose National Centre for Basic Sciences, Kolkata/IND; M. Havenith, Ruhr University Bochum/D

P 1.14 **Transformation of anharmonic potential energy surfaces for the efficient calculation of vibrational frequencies of isotopologues**
D. Oschetzki, P. Meier, G. Rauhut, Universität Stuttgart/D

P 1.15 **Vibrational multi-reference configuration interaction theory**
F. Pfeiffer, G. Rauhut, Universität Stuttgart/D

P 1.16 **Chemiluminescence of flames: Novel aspects for measurement and simulation**
J. Krüger, Universität Bielefeld/D

P 1.17 **UV Raman spectroscopy and force field analysis of silica supported vanadium oxide catalysts**
D. Nitsche, C. Hess, TU Darmstadt/D

P 1.18 **Spin density decomposition in the basis of paired orbitals**
S.P. Ruzankin, Boreskov Institute of Catalysis, Novosibirsk/RUS; I. Lyskov, Universität Düsseldorf/D; I.L. Zilberberg, Boreskov Institute of Catalysis, Novosibirsk/RUS

P 1.19 **New features in TRAVIS – Vibrational spectra from AIMD**
M. Brehm, M. Thomas, B. Kirchner, Universität Bonn/D

P 1.20 **Femtosecond pump-probe investigation of ortho-nitrophenol and its constitutional isomers in solution**
H.A. Ernst, T.J.A. Wolf, N. Gonzalez-Garcia, A.-U. Unterreiner, M. Olzmann, Karlsruher Institut für Technologie/D

P 1.21 **Novel organic hydrogen storage materials: Dehydrogenation of dodecahydro-*N*-ethylcarbazole on Pt and Pd model catalysts**
M. Amende, M. Sobota, S. Schernich, I. Nikiforidis, O. Höfert, W. Zhao, Y. Lykhach, C. Papp, W. Hieringer, M. Laurin, D. Assenbaum, P. Wasserscheid, H.-P. Steinrück, A. Görling, J. Libuda, FAU Erlangen-Nürnberg, Erlangen/D

P 1.22 **Adsorption of formic acid on ZnO (10-10) – An infrared reflection absorption spectroscopy study**
M. Buchholz, Q. Li, K. Fink, A. Nefedov, C. Wöll, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D

P 1.23 **The highly anharmonic systems FHF- and ClHCl-: Theory and experiment**
P. Sebald, A. Bargholz, R. Oswald, C. Stein, P. Botschwina, Universität Göttingen/D; K. Kawaguchi, Okayama University/J

P 1.24 **Spectroscopic properties of the c-C_6H_7 radical and its cation: A high-level theoretical study**
A. Bargholz, R. Oswald, P. Botschwina, Universität Göttingen/D

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M. Vaida, T.M. Bernhardt, Universität Ulm/D

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S. Pengel, B. Schönberger, A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D

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I. Halfpap, J. Plenge, E. Rühl, Freie Universität Berlin/D

P 1.28 **REMPI probing of IR-laser induced population transfer in NH_3 – First steps to measure parity violation in chiral molecules**
P. Dietiker, P. Miloglyadov, M. Quack, A. Schneider, G. Seyfang, ETH Zürich/CH

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P. Nuernberger, U. Selig, V. Dehm, V. Settels, M. Gsänger, B. Engels, F. Würthner, T. Brixner, Universität Würzburg/D

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H.V.L. Nguyen, RWTH Aachen/D

P 1.31 **Gas phase luminescence studies of chromophoric systems: Hypsochromic shifts, metal adducts, excited states lifetimes, comparison with theory**
J.F. Greisch, M.E. Harding, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D; W. Klopper, M.M. Kappes, D. Schooss, Karlsruhe Institute of Technology/D

P 1.32 **Rolled-up microtubes for light-matter interaction with colloidal quantum dots**
S. Kietzmann, C. Strelow, Universität Hamburg/D; A. Schramm, J.-P. Pettinen, T.V. Hakkarainen, Tampere University of Technology/FIN; A. Mews, T. Kipp, Universität Hamburg/D

P 1.33 **Modulation of Eu^{3+} emission by complexation of alkali metal cations to europium 9-hydroxylphenalen-1-one complexes in gas-phase**
J.F. Greisch, M.E. Harding, B. Schaefer, M. Ruben, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D; W. Klopper, M.M. Kappes, D. Schooss, Karlsruhe Institute of Technology/D

P 1.34 **Combined optical, electrical and scanning probe investigations of semiconductor nanowires**
D. Behn, C. Strelow, T. Kipp, A. Mews, Universität Hamburg/D

P 1.35 **Electrode potential dependent transformation of germanium/electrolyte interface in acidic medium: *In situ* electrochemical ATR-IR and DFT**
S. Nayak, P.U. Biedermann, S. Chakraborty, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D; R. Schmid, Ruhr-Universität Bochum/D; A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D

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T. Stolper, M. Andrejic, R.A. Mata, Universität Göttingen/D

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M. Vonderach, O.T. Ehrler, P. Weis, M.M. Kappes, Karlsruher Institut für Technologie/D

P 1.38 **Ion mobility, photoelectron spectroscopy, and collision induced dissociation of mono-, di- and trinuclear metal porphyrin multianions**
U. Schwarz, M. Vonderach, R. Kelting, K. Brendle, M. Kappes, P. Weis, Karlsruher Institut für Technologie/D

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S. Zinn, T. Betz, D. Schmitz, V.A. Shubert, M. Schnell, Center for Free-Electron Laser Science, Hamburg/D

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Y. Liang, Karlsruhe Institute of Technology/D; M. Bradler, Universität München/D; M. Klinger, Karlsruhe Institute of Technology/D; O. Schalk, Universität München/D; M.C. Balaban, T.S. Balaban, Aix Marseille Université/F; E. Riedle, Universität München/D; A.-N. Unterreiner, Karlsruhe Institute of Technology/D

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C.C. Pradzynski, F. Zurheide, T. Zeuch, Universität Göttingen/D

P 1.42 **A high resolution FTIR spectroscopic study of collisionally – cooled CHF_3**
I.B. Bolotova, O.N. Ulenikov, E.S. Bekhtereva, S. Albert, S. Bauerecker, H. Hollenstein, M. Quack, ETH Zürich/CH

P 1.43 **Ultrafast photoinduced dynamics of halogenated cyclopentadienes: Observation of geminate charge-transfer complexes in solution**
T.J.A. Wolf, Karlsruher Institut für Technologie/D; O. Schalk, Universität München/D; R. Radloff, Karlsruher Institut für Technologie/D; G. Wu, Chinese Academy of Sciences, Dalian/PRC; P. Lang, Universität München/D; A. Stolow, National Research Council, Ottawa/CDN; A.-N. Unterreiner, Karlsruher Institut für Technologie/D

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M. Lang, C. Schon, I. Fischer, Universität Würzburg/D

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O. Gromova, O. Ulenikov, E. Bekhtereva, S. Albert, Swiss Federal Institute of Technology Zurich/CH; S. Bauerecker, TU Braunschweig/D; H.-M. Niederer, M. Quack, Swiss Federal Institute of Technology Zurich/CH

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M.D. Kundrat, C.R. Jacob, Karlsruher Institut für Technologie/D

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R. Kannengießer, H.V.L. Nguyen, W. Stahl, RWTH Aachen University/D

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S. Fischer, E. Barsch, R. Ludwig, Universität Rostock/D; M. Bauer, TU Kaiserslautern/D

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A.P. Woodham, G. Meijer, Fritz-Haber-Institut der MPG, Berlin/D; A. Fielicke, TU Berlin/D

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F. Kollipost, A.V. Domanskaya, M.A. Suhm, Universität Göttingen/D

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A. Bihlmeier, W. Klopper, Karlsruher Institut für Technologie/D

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F. Kanal, S. Ruetzel, H. Lu, C. Lambert, T. Brixner, Universität Würzburg/D

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U. Pacher, T. Nagy, O. Armbruster, H. Pöhl, W. Kautek, Universität Wien/A

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D.A. Dewald, M.K. Jahn, D. Wachsmuth, J.-U. Grabow, Leibniz Universität Hannover/D; S. Mehrotra, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad/IND

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A. Tehlar, H.J. Wörner, ETH Zürich/CH

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V. Van, H. Mouhib, RWTH Aachen University/D

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G. Ahn-Ercan, ComputeChem, Saal an der Donau/D and Universität Regensburg/D

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V. Engel, M. Keß, A. Schubert, V. Settels, B. Engels, F. Würthner, Universität Würzburg/D; S. Lochbrunner, Universität Rostock/D; C. Meier, Universite Paul Sabatier, Toulouse/F

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M. Zimmer, S. Kruppa, M. Gerhards, TU Kaiserslautern/D

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N. Graf, Ruhr-Universität Bochum/D; D.P. Tew, University of Bristol/UK; C. Hättig, Ruhr-Universität Bochum/D

P 1.61 **Conformational space of the phycocyanobilin chromophore by *ab initio* spectroscopy**
T. Watermann, Universität Halle-Wittenberg, Halle (Saale)/D; H. Elgabarty, Freie Universität Berlin/D; D. Sebastiani, Universität Halle-Wittenberg, Halle (Saale)/D

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C.-N. Liu, B. Ozkaya, Universität Paderborn/D; S. Steves, P. Awakowicz, Ruhr-Universität Bochum/D; G. Grundmeier, Universität Paderborn/D

P 1.63 **High-resolution rotational spectroscopy of polyaromatic molecules and semiexperimental equilibrium structure of 1,3,4 oxadiazole**
M. Jahn, J.-U. Grabow, Leibniz Universität Hannover/D; D. McNaughton, P. Godfrey, Monash University, Victoria/AUS; E. Cocinero, Universidad del País Vasco, Bilbao/E; A. Lesarri, Universidad de Valladolid/E; J.-C. Guillemin, Ecole Nationale Supérieure de Chimie de Rennes/F; H.D. Rudolph, University of Ulm/D

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J. Jiang, M. Lewerenz, Universite Paris Est, Marne la Vallee Cedex 2/F

P 1.65 **NO^+ ions inside helium clusters: Structures, cohesive energies and size dependent vibrational frequency shifts**
D. Dominik, M. Lewerenz, Universite Paris Est, Marne la Vallee Cedex 2/F

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A. Frank, H.M. Möller, Universität Konstanz/D; T.E. Exner, Universität Tübingen/D

P 1.67 **Intrinsic fluorescence properties of rhodamine cations**
J.-F. Greisch, M.E. Harding, W. Klopper, M.M. Kappes, D. Schooss, Karlsruhe Institute of Technology/D

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M. Mladenovic, Université Paris Est, Marne la Vallée Cedex 2/F

P 1.69 **Metalated Hoogsteen binding in a nucleobase pair mimic by two-color IR dissociation spectroscopy and DFT calculations**
Y. Nosenko, F. Menges, C. Riehn, G. Niedner-Schatteburg, TU Kaiserslautern/D

P 1.70 **Semiclassical Wigner propagation as a numerical tool in molecular dynamics**
S. Ivanov, Universität Rostock/D; D. Marx, Ruhr-Universität Bochum/D; T. Dittrich, Universidad Nacional de Colombia, Bogotá D.C./CO

P 1.71 **Optical absorption spectra of small and medium coinage metal nanoclusters**
V. Grigoryan, M. Springborg, University of Saarland, Saarbrücken/D; H. Minassian, A.I. Alikhanyan National Science Laboratory, Yerevan/ARM; A. Melikyan, Russian-Armenian State University, Yerevan/ARM

P 1.72 **The dynamic structure of the benzene dimer – A floppy symmetric top**
M. Schnell, Center for Free-Electron Laser Science, Hamburg/D; P.R. Bunker, National Research Council, Ottawa/CDN; U. Erlekam, G. von Helden, Fritz-Haber-Institut der MPG, Berlin/D; J.-U. Grabow, Leibniz-Universität Hannover/D; G. Meijer, Fritz-Haber-Institut der MPG, Berlin/D; A. van der Avoird, Radboud Universiteit Nijmegen/NL

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S.I. Bokarev, S. Ivanov, O. Kühn, University of Rostock/D

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F. Latorre, University of Vienna/A; J. Guthmuller, Gdansk University of Technology/PL; P. Marquetand, L. González, University of Vienna/A

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K. Meister, Ruhr University Bochum/D; Y. Xu, Unviversity of Nevada, Reno/USA; S. Ebbinghaus, Ruhr University Bochum/D; J. Duman, University of Notre Dame/USA; A. DeVries, M. Gruebele, University of Illinois, Urbana-Champaign/USA; D. Leitner, University of Nevada, Reno/USA; M. Havenith, Ruhr University Bochum/D

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S.A. Baeurle, E. Peter, B. Dick, Universität Regensburg/D

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B.R. Brückner, A. Pietuch, A. Janshoff, Universität Göttingen/D

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N. Bohn, T. Hadler, Universität Hamburg/D

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K. Kartaschew, M. Mischo, S. Baldus, E. Bründermann, P. Awakowicz, M. Havenith, Ruhr-Universität Bochum/D

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E. Herman, T. Kottke, Universität Bielefeld/D; M. Sachse, P. Kroth, Universität Konstanz/D

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E. Edengeiser, J.W. Lackmann, S. Schneider, F. Jarzina, S. Brinckmann, E. Steinborn, E. Bründermann, J. Benedikt, J.E. Bandow, M. Havenith, Ruhr-Universität Bochum/D

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J. Pecher, R.A. Mata, Universität Göttingen/D

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F. Schulz, N.G. Bastús, T. Vossmeyer, H. Weller, Universität Hamburg/D

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G. Bekcioglu, C. Allolio, D. Sebastiani, Universität Halle-Wittenberg, Halle (Saale)/D

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C. Wolter, Universität Hamburg/D

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J. Dielmann, V. Conti Nibali, E. Bründermann, Ruhr-Universität Bochum/D; B. Born, M. Grossmann, I. Sagi, The Weizmann Institute of Science, Rehovot/IL; M. Havenith, Ruhr-Universität Bochum/D

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V. Conti Nibali, Ruhr-Universität Bochum/D; M. Heyden, University of California, Irvine, CA/USA; J. Dielmann, Ruhr-Universität Bochum/D; M. Grossman, B. Born, T. Tworowski, I. Sagi, The Weizmann Institute of Science, Rehovot/IL; M. Havenith, Ruhr-Universität Bochum/D

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D. Nordmeyer, N. Fendel, Freie Universität Berlin/D; S. Ahlberg, F. Rancan, A. Vogt, J. Lademann, Charité – Universitätsmedizin, Berlin/D; C. Greulich, M. Köller, Ruhr-Universität Bochum/D; J. Diendorf, M. Epple, Universität Duisburg-Essen, Essen/D; J. Raabe, Paul Scherrer Institute, Villigen-PSI/CH; C. Graf, E. Rühl, Freie Universität Berlin/D

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M. Senske, Ruhr-Universität Bochum/D; B. Born, The Weizmann Institute of Science, Rehovot/IL; M. Mischo, Ruhr-Universität Bochum/D; A. Bitler, S. Cohen, The Weizmann Institute of Science, Rehovot/IL; L. Troeberg, Imperial College London/UK; G. Opdenakker, Katholieke Universiteit Leuven/B; I. Sagi, The Weizmann Institute of Science, Rehovot/IL; M. Havenith, Ruhr-Universität Bochum/D

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M. Kahse, R. Winter, TU Dortmund/D

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M. Erlkamp, S. Grobelny, R. Winter, TU Dortmund/D

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B. Lechner, S. Werner, A. Achilles, H. Ebert, C. Tschierske, C. Bacia, K. Saalwächter, A. Blume, University of Halle-Wittenberg, Halle (Saale)/D

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M. Alles, C. Christophis, Universität Heidelberg/D; M.E. Callow, University of Birmingham/UK; A. Rosenhahn, Universität Heidelberg/D

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R. Horeis, C. Dosche, T. Klüner, University of Oldenburg/D; B. Rogez, E. Boer-Duchemin, G. Comtet, G. Dujardin, University of Paris South/F; J. Christoffers, K. Al-Shamery, University of Oldenburg/D

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M. Langeloth, TU Darmstadt/D; Y. Masubuchi, Kyoto University/J; M.C. Böhm, F. Müller-Plathe, TU Darmstadt/D

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F. Bergler, F. Schöppler, T. Hertel, Universität Würzburg/D

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M. Zugermeier, M. Chen, H.-J. Drescher, J.M. Gottfried, Universität Marburg/D

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I. Hoffmann, TU Berlin/D and ILL, Grenoble/F; B. Farago, ILL, Grenoble/F; M. Gradzielski, TU Berlin/D

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M. Pfeifle, M. Olzmann, Karlsruher Institut für Technologie/D

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L. Genthner, P. Friese, J. Kiecherer, T. Bentz, M. Olzmann, Karlsruher Institut für Technologie/D

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J. Kiecherer, B. Derstroff, M. Magar, S. Faas, T. Bentz, U. Maas, M. Olzmann, Karlsruher Institut für Technologie/D

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M. Zühlke, D. Riebe, C. Brendler, T. Beitz, H.-G. Löhmannsröben, Universität Potsdam/D; A. Charvat, B. Abel, Leibniz-Institut für Oberflächenmodifikation (IOM), Leipzig/D

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J. Mohrbach, C. Merkert, L. Barzen, M. Tombers, J. Hewer, G. Niedner-Schatteburg, TU Kaiserslautern/D

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P. Kube, B. Frank, R. Schlögl, A. Trunschke, Fritz-Haber-Institut der MPG, Berlin/D

P 4.08 **Highly selective low temperature methane conversion on free gold dimers**
S.M. Lang, T.M. Bernhardt, Universität Ulm/D

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I. Herber, O.P. Balaj, M.K. Beyer, Universität zu Kiel/D

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T. Uhlemann, K.-M. Weitzel, Universität Marburg/D

P 4.11 **Adsorption kinetics of multiply charged metal porphyrin anions at low temperatures**
T. Karpuschkin, O. Hampe, M.M. Kappes, Karlsruhe Institute of Technology/D

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A.V. Domanskaya, F. Kollipost, M.A. Suhm, Universität Göttingen/D

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K. Moshammer, Universität Bielefeld/D; D. Mayer, H. Pitsch, RWTH Aachen/D; K. Kohse-Höinghaus, Universität Bielefeld/D

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P. Kraus, A. Gijsbertsen, H.J. Wörner, ETH Zürich/CH

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Y. Chang, J. Küpper, Center for Free-Electron Laser Science, Hamburg/D; D. Rösch, S. Willitsch, Universität Basel/CH

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W. Friedrich, F. Schulz, K. Hoppe, H. Weller, University of Hamburg/D

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C. Niedrig, W. Menesklou, S.F. Wagner, E. Ivers-Tiffée, Karlsruhe Institute of Technology/D

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M. Wächtler, J. Kübel, R. Siebert, A. Winter, U.S. Schubert, B. Dietzek, University of Jena/D

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Y. Pang, Saarland University, Saarbrücken/D

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Y. Dong, Saarland University, Saarbrücken/D

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J. Zischang, M.A. Suhm, Universität Göttingen/D

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M. Grüßer, X. Ma, R. Schuster, Karlsruher Institut für Technologie/D

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R. Haunschild, Karlsruher Institut für Technologie/D; D. Mukherjee, Indian Association for the Cultivation of Science, Kolkata/IND; W. Klopper, Karlsruher Institut für Technologie/D

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M. Schmitt, Saarland University, Saarbrücken/D

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S. Kittler, J. Poppe, S.G. Hickey, A. Eychmüller, TU Dresden/D

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S. Donets, A. Pershin, S.A. Baeurle, University of Regensburg/D

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E. Huber, Universität Hamburg/D

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F. Heß, H. Over, Universität Gießen/D

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F. Heß, H. Over, Universität Gießen/D

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B. Over, B. Rathke, S. Will, Universität Bremen/D

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D. Emmrich, H. Vieker, A. Beyer, Universität Bielefeld/D

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F. Conti, A. Majerus, S. Willbold, W. Lehnert, C. Korte, Forschungszentrum Jülich GmbH/D

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S. Merz, Center for Free-Electron Laser Science, Hamburg/D and Max-Planck-Institut für Kernphysik, Heidelberg/D; N. Vanhaecke, G. Meijer, Fritz-Haber-Institut der MPG, Berlin/D; M. Schnell, Center for Free-Electron Laser Science, Hamburg/D and Max-Planck-Institut für Kernphysik, Heidelberg/D

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A. Petrov, K. Kurth, T. Vossmeyer, H. Weller, Universität Hamburg/D

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D. Wachsmuth, D.A. Dewald, M.K. Jahn, J.-U. Grabow, Leibniz Universität Hannover/D

P 5.24 **Laser-induced electrochemical de- and repassivation investigations on plasma-oxidized aluminium alloys**
T. Nagy, U. Pacher, A. Giesriegl, L. Soyka, G. Trettenhahn, W. Kautek, Universität Wien/A

P 5.25 **Modeling solute polarizability in 3D integral equation theory**
R. Frach, J. Heil, F. Hoffgaard, S. Egbers, S.M. Kast, TU Dortmund/D

P 5.26 **Development of a perturbative QM/MM Monte Carlo method for the study of molecules in solution**
J.C. Oliveira, R.A. Mata, Universität Göttingen/D

P 5.27 **Predicting ion selectivity of biological and synthetic nanopores by molecular dynamics simulations and 3D integral equation theory**
L.M. Henkes, F. Mrugalla, R. Frach, S.M. Kast, TU Dortmund/D

P 5.28 **Towards a thermodynamically consistent, quantitatively accurate integral equation theory**
D. Tomazic, M. Urban, S.M. Kast, TU Dortmund/D

P 5.29 **Reference beams from dense fluids**
W. Christen, B.-G. Chen, Humboldt-Universität zu Berlin/D

P 5.30 **Methanol synthesis from molecular dynamics**
J. Frenzel, D. Marx, Ruhr-Universität Bochum/D

P 5.31 **Photoluminescence spectroscopy of individual CdSe quantum wires at low temperatures**
A. Reich, D. Franz, Universität Hamburg/D; Z. Wang, Universität Zürich/CH; T. Kipp, A. Mews, Universität Hamburg/D

P 5.32 **A multivariate method to disentangle complex spectra**
T. Gladytz, E. Lugovoy, Universität Leipzig/D; K. Siefermann, B. Abel, Leibniz Institut für Oberflächenmodifizierung, Leipzig/D

P 5.33 **Towards attosecond time-resolved molecular spectroscopy using laser-induced electron diffraction**
S.G. Walt, T. Karg, H.J. Wörner, ETH Zürich/CH

P 5.34 **CO oxidation over flame made manganese oxide catalysts**
M.T. Tepluchin, M.C. Casapu, Karlsruher Institut für Technologie/D; D.P. Pham, L.M. Mädler, Universität Bremen/D; J.-D.G. Grunwaldt, Karlsruher Institut für Technologie/D

P 5.35 **Combined *in situ* XAS and DRIFTS measurements of CO/NO-oxidation over Pt-based diesel oxidation catalysts**
A. Gänzler, A. Boubnov, M. Casapu, H. Lichtenberg, J.-D. Grunwaldt, Karlsruher Institut für Technologie/D

P 5.36 **A low scaling PNO-MP2 method for investigation of dispersion interaction in large systems**
G. Schmitz, B. Helmich, C. Hättig, Ruhr-Universität Bochum/D

P 5.37 **Using rapid-scan IR-techniques for examining water reduction**
B. Hoffmann, Universität Rostock/D; E. Barsch, Leibniz-Institut für Katalyse e.V., Rostock/D; S. Fischer, R. Ludwig, Universität Rostock/D

P 5.38 **Thermodynamics of temperature induced self-aggregation processes with variable stoichiometry**
L. Chiappisi, TU Berlin/D; G. Lazzara, Universitá degli Studi di Palermo/I; M. Gradzielski, TU Berlin/D; S. Milioto, Universitá degli Studi di Palermo/I

P 5.39 **Semiconductor nanoparticles made at the plasma/ionic liquid interface**
N. Spitczok von Brisinski, O. Höfft, F. Endres, TU Clausthal, Clausthal-Zellerfeld/D

P 5.40 **Imaging catalysts by hard X-rays: New opportunities of X-ray tomography and ptychography in the nanoscale**
G. Hofmann, Karlsruher Institut für Technologie/D; R. Hoppe, TU Dresden/D; J. Reinhardt, C.G. Schroer, TU Dreseden/D; J.-D. Grunwaldt, Karlsruher Institut für Technologie/D

P 5.41 **In operando X-ray absorption spectroscopy studies at the ANKA synchrotron light source**
H. Lichtenberg, A. Boubnov, S. Mangold, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D; M. Casapu, D. Doronkin, H.W. Pereira de Carvalho, Karlsruher Institut für Technologie/D; M. Schubert, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D; J.-D. Grunwaldt, Karlsruher Institut für Technologie/D

P 5.42 **New synthetic route towards nanostructured dye-sensitized NiO layers and spectroscopic investigations**
M. Bräutigam, P. Weyell, Friedrich-Schiller-University Jena/D; J. Popp, Institute of Photonic Technology Jena/D; F.H. Schacher, Friedrich-Schiller-University Jena/D; B. Dietzek, Institute of Photonic Technology Jena/D

Interfaces

P 6.01 **Surface activated dedeuteration of deuterofullerenes**
S. Ulas, P. Weis, A. Böttcher, M. Kappes, Karlsruher Institut für Technologie/D

P 6.02 **Thermal analysis of heat transfer from V2A-steel surface**
M. Schmitt, Saarland University, Saarbrücken/D

P 6.03 **Determination of retention forces by contact angle measurements on rough solid surfaces using sessile drop methods**
M. Schmitt, F. Heib, Saarland University, Saarbrücken/D

P 6.04 **Morphology of photo-switchable azobenzene monolayers**
S. Riaz, G. Friedrichs, University of Kiel/D

P 6.05 **Reversible switching between Eu(II) and Eu(III) in ultrathin films**
S. Matz, M. Ahlf, J. Bruns, M. Wickleder, K. Al-Shamery, University Oldenburg/D

P 6.06 **Steady state evaporation of nanodroplet using non-equilibrium molecular dynamics simulations**
J. Zhang, F. Leory, F. Müller-Plathe, TU Darmstadt/D

P 6.07 **Whispering gallery modes in ZnO microspheres for sensitive optical spectroscopy**
R. Moirangthem, A. Erbe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf/D

P 6.08 **Reactive wetting effects of silicon on silicon dioxide**
L.D. Alphei, V. Becker, R. Grotjahn, R. Janhsen, J.A. Becker, Leibniz Universität Hannover/D

P 6.09 **Electrochemical studies of CrAlN coatings deposited by high power pulsed magnetron sputtering**
M. Wiesing, O. Ozcan, C. Kunze, S. Waschke, Universität Paderborn/D; R. Brugnara, K. Bobzin, RWTH Aachen/D; G. Grundmeier, Universität Paderborn/D

P 6.10 **Emission properties of quantum dots affected by the ligand shell – Theory and experiment**
S. Leubner, TU Dresden/D; S. Hatami, BAM Bundesanstalt für Materialforschung und -prüfung, Berlin/D; T. Lorenz, J.-O. Joswig, N. Gaponik, TU Dresden/D; U. Resch-Genger, BAM Bundesanstalt für Materialforschung und -prüfung, Berlin/D; A. Eychmüller, TU Dresden/D

P 6.11 ***Multi in situ* spectroscopy of CeO_2 and Au/CeO_2**
M. Lohrenscheit, C. Hess, TU Darmstadt/D

P 6.12 **Interaction of water with rutile (110)**
J. Mitschker, Th. Klüner, Universität Oldenburg/D

P 6.13 **Functional single-layer graphene sheets by conversion of organic monolayers**
D.G. Matei, N.-E. Weber, Universität Bielefeld/D; S. Kurasch, Universität Ulm/D; S. Wundrack, M. Woszczyna, M. Grothe, T. Weimann, F. Ahlers, R. Stosch, Physikalisch-Technische Bundesanstalt, Braunschweig/D; U. Kaiser, Physikalisch-Technische Bundesanstalt, Ulm/D; A. Turchanin, Universität Bielefeld/D

P 6.14 **Vibrational sum frequency generation study of the 2D phase behavior of Langmuir monolayers**
J. Kleber, G. Friedrichs, Universität zu Kiel/D

P 6.15 **What is the contact angle of water on graphene?**
F. Taherian, V. Marcon, N.F.A. van der Vegt, F. Leroy, TU Darmstadt/D

P 6.16 ***In situ* DRIFTS on alkali salt-modified supported catalysts for methanol steam reforming**
A. Kaftan, M. Kusche, B. Morain, H. Niedermeyer, P. Wasserscheid, M. Laurin, J. Libuda, FAU Erlangen-Nürnberg, Erlangen/D

P 6.17 **Interaction of CO with rutile (110)**
W. Dononelli, Th. Klüner, Universität Oldenburg/D

P 6.18 **Ferrocene ultrathin films on NaCl(100)**
B. Vogt, J. Vogt, Universität Magdeburg/D

P 6.19 **LEED structure analysis of CO and N_2 adsorbed on the NaCl(100) surface**
B. Vogt, J. Vogt, Universität Magdeburg/D

P 6.20 **Surface functionalization by ionic liquids: Ultrathin films of [5-oxo-C_6C_1Im][Tf_2N] on CeO_{2-x}/Cu(111)**
S. Schernich, Y. Lykhach, V. Wagner, N. Taccardi, P. Wasserscheid, H.-P. Steinrück, M. Laurin, J. Libuda, FAU Erlangen-Nürnberg, Erlangen/D; N. Tsud, T. Skála, V. Matolín, Charles University, Prague/CZ; K.C. Prince, Synchrotrone Trieste/I

P 6.21 **Photothermally induced bromination of organic monolayers on graphite**
M. Przyklenk, S. Franzka, N. Hartmann, Universität Duisburg-Essen, Essen/D

P 6.22 **Adhesion force investigations of micro-particles on polymer surfaces**
J. Colson, O. Armbruster, S. Koprivica, W. Kautek, Universität Wien/A

P 6.23 **Importance of spatial resolution in catalytic reactors: Gradients in the catalyst structure during the partial oxidation of methane**
A. Rochet, G. Hofmann, S. Baier, J.D. Grunwaldt, Karlsruhe Institute of Technology/D

P 6.24 **Probing shallow trapped electron states and related processes of TiO_2 with UHV-IRRAS**
H. Sezen, C. Natzeck, A. Nefedov, C. Wöll, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D

P 6.25 **Operando-spectroscopic study on the structure-function relationship of Pd-doped SnO_2 gas sensors**
H.W. Pereira de Carvalho, Karlsruhe Institute of Technolgy/D; D. Degler, M. Hübner, J. Rebholz, B. Barsan, W. Weimar, University of Tübingen/D; D.K. Pham, L. Mädler, Universität Bremen/D; J.D. Grunwaldt, Karlsruhe Institute of Technolgy/D

P 6.26 **A setup for measuring adsorption isotherms on individual single-wall carbon nanotubes**
T. Hain, T. Hertel, Universität Würzburg/D

P 6.27 **Kinetic studies into the initial oxidation of Ru(0001) to RuO_2**
J.C. Goritzka, B. Herd, D. Langsdorf, A. Farkas, S. Rohrlack, H. Over, Universität Gießen/D; O. Balmes, ESRF, Grenoble/F; A. Pietzsch, J. Knudsen, J. Schnadt, N. Johansson, E. Lundgren, J.N. Andersen, University of Lund/S; J.I. Flege, Universität Bremen/D

P 6.28 **Systematische Studien zur Funktionalisierung anisotroper Goldnanopartikel**
F. Brenner, C. Graf, Freie Universität Berlin/D

P 6.29 **Adsorption and diffusion in thin films of nanoporous metal-organic frameworks: Ferrocene in SURMOF $Cu_2(bdc)_2$(dabco)**
L. Heinke, H. Gliemann, C. Wöll, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D

P 6.30 **H and D/ r-TiO_2(110): Adsorption, desorption and uptake**
N. Osterloh, Ruhr-Universität Bochum/D; F. Traeger, Westfälische Hochschule, Recklinghausen/D; H.-W. Becker, D. Rogalla, Ruhr-Universität Bochum/D

Solid State

P 7.01 **Local structure and oxygen dynamics in Ti/Ta doped CeO_2 investigated by ^{17}O NMR spectroscopy**
R. Heinzmann, I. Issac, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D; J.-P. Eufinger, University of Gießen/D; G. Ulbrich, TU Berlin/D; J. Janek, University of Gießen/D; M. Lerch, TU Berlin/D; S. Indris, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D

P 7.02 **Synthesis, characterization and electrochemical properties of nanosized $Fe_{2-x}Al_xO_3$ (x=0,0.2,0.3,0.5,0.7,1)**
I. Issac, R. Heinzmann, M. Kaus, S. Indris, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D

P 7.03 **Synthesis and spectroscopy of carbon nanowalls and few-layered graphene sheets with deposited metal nanoparticles**
M. Höltig, A. Mews, Universität Hamburg/D

P 7.04 **C_{58} materials: Thermally modified mechanical properties**
S. Ulas, S. Bundschuh, Karlsruher Institut für Technologie/D; S. Jester, Universität Bonn/D; C. Eberl, H. Hölscher, A. Böttcher, M. Kappes, Karlsruher Institut für Technologie/D

P 7.05 **Relationship of nanoparticle morphology and superstructure ordering of gold-mesocrystals**
D. Haubold, L. Liebscher, TU Dresden/D; P. Simon, Max Planck Institute for Chemical Physics of Solids, Dresden/D; S.G. Hickey, A. Eychmüller, TU Dresden/D

P 7.06 **Cathodoluminescence of gold surfaces patterned by electron beam lithography using self-assembled monolayers of alkanethiolates as resists**
X. Ma, M. Grüßer, R. Schuster, Karlsruher Institut für Technologie/D

P 7.07 **Cadmium doped lead selenide nanorods emitting in the imaging window**
C. Bothe, A. Kornowski, H. Weller, University of Hamburg/D

P 7.08 **Synthesis of rare-earth trifluoride nanoparticles based on small sacrificial particles**
A.N. Raj, V. Jendrock, T. Rinkel, M. Haase, Universität Osnabrück/D

P 7.09 **Enhanced photo-luminescence of $NaEuF_4$ nanocrystals through ligands with broadband absorption and high extinction coefficents**
S. Dühnen, B. Voß, M. Haase, Universität Osnabrück/D

P 7.10 **Monodispersed Sub-10 nm sized $NaLnF_4$ nanocrystals of the lighter lanthanides La, Ce, Pr and Nd**
A. Naduviledathu Raj, S. Dühnen, M. Haase, University of Osnabrück/D

P 7.11 **Core-shell-structures of $CuInS_2$/ZnS nanorods and $CuInS_2$-Au-linking via polyelectrolytes**
B. Kempken, J. Parisi, J. Kolny-Olesiak, Universität Oldenburg/D

P 7.12 **Controlling the optical properties of quantum-dot-based gels**
A. Wolf, TU Dresden/D; V. Lesnyak, Istituto Italiano di Tecnologia, Genova/I; N. Gaponik, A. Eychmüller, TU Dresden/D

P 7.13 **Größenabhängige Eigenschaften polarer oxidischer Nanokristalle**
K. Kömpe, M. Imlau, Universität Osnabrück/D

P 7.14 **Synthese von naturnahem Hydroxylapatit**
M. Plein, A. Schlepphorst, D. Stoppel, K. Thierbach, K. Kömpe, Universität Osnabrück/D

P 7.15 **Highly sensitive absorption and loss spectroscopy**
W. Paa, C. Mühlig, T. Zeuner, Institut für Photonische Technologien e.V., Jena/D

P 7.16 **Untersuchung der Durchmischung von $NaEuF_4$ und $NaYF_4$ Vorläuferpartikeln zu Eu^{3+}-dotierten ß-$NaYF_4$**
F. Carl, B. Voß, M. Haase, Universität Osnabrück/D

P 7.17 **Synthesis of highly luminescent zinc containing indium phosphide nanoparticles**
G.M. Stachowski, S.G. Hickey, A. Eychmüller, TU Dresden/D

P 7.18 **CO oxidation by supported iron catalysts: A multi-dimensional spectroscopic approach**
R. Schoch, M. Bauer, TU Kaiserslautern/D

P 7.19 **Synthesis, characterisation and surface modification of III-V nanocrystals for biomedical applications**
S. Wölper, A. Kornowski, H. Weller, University of Hamburg/D

P 7.20 **Oxygen diffusion in mayenite**
M. Teusner, R.A. De Souza, RWTH Aachen/D; H. Krause, S.G. Ebbinghaus, Universität Halle-Wittenberg, Halle (Saale)/D; M. Martin, RWTH Aachen/D

P 7.21 **Investigation of the formation mechanism of ß-Ga_2O_3**
H. Schraknepper, R.A. De Souza, M. Martin, RWTH-Aachen University/D

P 7.22 **Low-temperature luminescence study of novel NaYF4-based upconversion nanoparticles (UCNP) co-doped with (Gd:Yb:Er)**
D. Klier, Universität Potsdam/D; S.-H. Kung, E. Rühl, Freie Universität Berlin/D; M. Kumke, Universität Potsdam/D

P 7.23 **Natural chabazite for NO_x-removal – Looking at the active sites using *in situ* X-ray absorption spectroscopy**
T. Günter, M. Casapu, J.-D. Grunwaldt, Karlsruher Institut für Technologie/D

P 7.24 **Time-resolved fluorescence spectroscopy of individual semiconductor dot-in-a-rod nanocrystals at low temperature**
Ch. Strelow, E. Huber, T. Kipp, A. Mews, Universität Hamburg/D

P 7.25 **Size and shape control of copper tin sulfide nanocrystals**
M. Kruszynska, J. Parisi, J. Kolny-Olesiak, Universität Oldenburg/D

P 7.26 **Mechanochemistry: From mechanical degradation to novel materials properties**
V. Sepelák, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D; K.D. Becker, TU Braunschweig/D

P 7.27 **CO oxidation over flame made manganese oxide catalysts**
M. Tepluchin, M. Casapu, Karlsruher Institut für Technologie/D; D.K. Pham, L. Mädler, University of Bremen/D; J.-D. Grunwaldt, Karlsruher Institut für Technologie/D

P 7.28 **Structure and reducibility of a Fe/Al_2O_3 catalyst for SCR studied by *in situ* Fe K-edge XAFS spectroscopy**
A. Boubnov, H. Lichtenberg, Karlsruher Institut für Technologie/D; S. Mangold, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen/D; J.-D. Grunwaldt, Karlsruher Institut für Technologie/D

P 7.29 **Impact of mixed cation effect on Li diffusivity in channel-structured $Li_xNa_{2-x}Ti_6O_{13}$**
K. Volgmann, P. Heitjans, Leibniz Universität Hannover/D

P 7.30 **Luminescence of Eu^{2+} in $LiSrH_3$, $LiBaH_3$ and the corresponding deuterides**
N. Kunkel, M. Springborg, Universität des Saarlandes, Saarbrücken/D; H. Kohlmann, Leipzig University/D; A. Meijerink, Utrecht University/NL

P 7.31 **Amorphe Stoffe aus kleinen organischen Molekülen**
H.K. Cammenga, TU Braunschweig/D; K. Gehrich, Südzucker AG, Offstein/D

Liquid State

P 8.01 **Investigation of Li diffusion and transference numbers of ionic liquid based electrolytes by ^{7}Li NMR**
R. Heinzmann, A. Hofmann, M. Schulz, S. Indris, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen/D

P 8.02 **Hydration of the osmolyte ectoine in water and aqueous NaCl**
A. Eiberweiser, A. Nazet, T. Rück, R. Buchner, University of Regensburg/D

P 8.03 **Proton conductivity in MIL53Al-MOF structures**
E. Eisbein, J.-O. Joswig, G. Seifert, TU Dresden/D

P 8.04 **Thermostatted ice growth from supercooled water in simulations follows Wilson-Frenkel kinetics**
V.C. Weiss, T. Frauenheim, University of Bremen/D

P 8.05 **Quantum optics and photoacids**
M. Vester, Saarland University, Saarbrücken/D

P 8.06 **Ultrafast photoinduced dynamics of the 3,6-diaminoacridinium derivative ATTO 465 in liquids**
J. Arden-Jacob, K.H. Drexhage, S.I. Druzhinin, M. Ekimova, O. Flender, T. Lenzer, K. Oum, Universität Siegen/D; M. Scholz, MPI für biophysikalische Chemie, Göttingen/D

P 8.07 **A full-dimensional and reactive neural network potential for water clusters based on density-functional theory**
T. Morawietz, K.N. Suresh, J. Behler, Ruhr-Universität Bochum/D

P 8.08 **Extracting THz features of ions: Experimental and theoretical investigation of lanthanides hydration**
V. Sharma, Ruhr University Bochum/D

P 8.09 **Vertical photoionization of liquid-to-supercritical ammonia: Thermal effects on the valence-to-conduction band gap**
J. Urbanek, J. Lindner, P. Vöhringer, Universität Bonn/D

P 8.10 **Utilization of N-methyl-6-oxyquinolinium betaine for probing inter- and intramolecular interactions in ionic liquids**
S. Schmode, Universität Rostock/D; N.P. Ernsting, Humboldt-Universität zu Berlin/D; R. Ludwig, Universität Rostock/D

P 8.11 **Recombination dynamics of solvated electrons in liquid-to-supercritical methanol**
A. Gehrmann, J. Lindner, P. Vöhringer, Universität Bonn/D

P 8.12 **Interaction power of anions in ionic liquids converts solvent separated into contact ion pairs**
M. Strauch, F. Kubatzki, C. Roth, R. Ludwig, Universität Rostock/D

P 8.13 **Physicochemical properties of glyme-lithium salt mixtures – Experiments and simulations**
A. Bonsa, A. Appelhagen, J.K. Lehmann, R. Ludwig, Universität Rostock/D

P 8.14 **Polarisability in ionic liquids**
C. Schröder, M. Schmollngruber, O. Steinhauser, Universität Wien/A

P 8.15 **Femtosecond two-dimensional infrared spectroscopy of thiocyanate anions in water**
D. Czurlok, D. Ehmer, J. Lindner, P. Vöhringer, Universität Bonn/D

P 8.16 **Investigation of ferrous and ferric ions in aqueous solution via terahertz spectroscopy**
F. Böhm, V. Sharma, G. Schwaab, M. Havenith, Ruhr-Universität Bochum/D

P 8.17 **Comparison of sonication and shear-mixing for the dispersion of single-wall carbon nanotubes**
T. Hefner, S. Stahl, Universität Würzburg/D; D.E. Resasco, University of Oklahoma, Norman/USA; T. Hertel, Universität Würzburg/D

P 8.18 **Carbon 1s binding energies of hydrated alcohols and acids**
I. Jordan, H.J. Wörner, J.A. van Bokhoven, M.A. Brown, ETH Zürich/CH

P 8.19 **Dendritic freezing of supercooled water droplets: Study of electric charge separation**
T. Buttersack, S. Bauerecker, TU Braunschweig/D

P 8.20 **Spectroscopic analyses on the excited states and reactivity of homo- and hetero nuclear transition metal complexes in solution**
A. Grün, R. Schepper, Y. Schmitt, TU Kaiserslautern/D; F. Armbruster, F. Walz, S. Styra, S. Gonzalez-Gallardo, Karlsruher Institut für Technologie/D; K. Salih, W.R. Thiel, TU Kaiserslautern/D; F. Breher, Karlsruher Institut für Technologie/D; M. Gerhards, TU Kaiserslautern/D

P 8.21 **Ultrafast reversible switching dynamics and solvation shell rearrangements of a photo-switchable catalyst tracked from femto to nanoseconds**
M. Pescher, L. Van Wilderen, Universität Frankfurt/D; S. Gruetzner, S. Hecht, Humboldt-Universität zu Berlin, Berlin/D; J. Bredenbeck, Universität Frankfurt/D

P 8.22 **Molecular association in statistical thermodynamics**
W. Schröer, Universität Bremen/D

P 8.23 **The phase behavior of mixtures of 1-alkyl-3-methylimidazonium bis(trifluoromethylsulfonyl)amides with *n*-alkyl-alcohols**
B. Rathke, W. Schröer, Universität Bremen/D

Electrochemical Interfaces

P 9.01 **Recycling of tantalum capacitors using an ionic liquid**
L. Spitczok von Brisinski, D. Goldmann, F. Endres, TU Clausthal, Clausthal-Zellerfeld/D

P 9.02 **Absorption and photoluminescence-spectroscopy of single-wall carbon nanotubes under potentiostatic control**
H. Hartleb, C.L. Rider-Dobson, T. Hertel, Universität Würzburg/D

P 9.03 **Microcalorimetric study on the mechanism of electrochemical deposition and dissolution of silver**
K.R. Bickel, R. Schuster, Karlsruher Institut für Technologie/D

P 9.04 **Electrochemical tuning of magnetism of γ-Fe_2O_3 nanoparticles studied by SQUID magnetometry combined with *in situ* cyclic voltammetry**
S. Topolovec, TU Graz/A; H. Krenn, Universität Graz/A; R. Würschum, TU Graz/A

P 9.05 **Electrochemical adsorption and deposition processes studied by time-resolved surface plasmon resonance**
A.E. Timm, D. Nattland, R. Schuster, Karlsruher Institut für Technologie/D

P 9.06 ***In situ*-Ramanspektroskopie an Lithium-Ionen-Batterien**
T. Groß, C. Hess, TU Darmstadt/D

Thursday, May 9, 2013

19:30 – 22.00 **Welcome Reception** (Festsaal Studentenwerk KIT)

Opening dinner with hot and cold buffet and beverages.
Admission is free, but advance online registration is requested.
Please tick the appropriate box on the online registration form.

Friday, May 10, 2013

10:00 – 11:30 **Guided Tour of the "Bundesgerichtshof"** (Federal Court of Justice in Karlsruhe)
(Language: German)

Admission is free, but advance registration is required, since the number of participants is limited to 35 persons.

Registrations should be sent directly to Mrs. Dagmar Wagner (bunsen2013@ipc.kit.edu) **before April 19, 2013.**

PLEASE NOTE: You will must provide a copy of your identity card or passport when registering. Please also bring the document with you by the visit.

18:00 – 22:00 **Poster Session**

The Poster Session allows for in-depth exchange of latest research achievements and developments in an informal atmosphere while enjoying a snack and drink with friends and colleagues.
Admission is free, but advance online registration is requested. Please tick the appropriate box on the online registration form.

Saturday, May 11, 2013

10:00 – 12:00 **Guided Walking Tour of Karlsruhe**
(Language: English)

Price: 10 € (incl. 19% VAT)
Registrations should be sent directly to Mrs. Dagmar Wagner (bunsen2013@ipc.kit.edu) **before April 19, 2013.**

PLEASE NOTE: Tickets for the Guided Walking Tour can be cancelled without charges **before April 19, 2013**. Cancellations received thereafter will not be eligible for any refund.

From 19:00 **Conference Dinner at ZKM Karlsruhe** (Foyer)
ZKM – Zentrum für Kunst und Medientechnologie Karlsruhe (Center for Art and Media Karlsruhe)
Lorenzstraße 19, 76135 Karlsruhe

Price: 55 € (incl. 19% VAT), incl. food and drinks
The dinner price also includes a **"Bunsentagung" guided tour through the ZKM from 18:00 on**.
Additionally, conference dinner participants will have free access to the museum all day on Saturday.
Advance online registration for the conference dinner and the ZKM guided tour is required.
Please tick the appropriate box on the online registration form.

PLEASE NOTE: Conference Dinner tickets can be cancelled without charges **before April 5, 2013**.
Cancellation received thereafter will not be eligible for any refund.

The Karlsruhe tourism department offers a variety of cultural events and visitors programmes.
For further information please consult the website www.karlsruhe-tourismus.de.

REGISTRATION FEES[1)]

Registration fees until March 27, 2013

Personal Members of the German Bunsen Society	110 €
Non-Members	140 €
Students[2)] (proof of status required, no Ph.D. students)	35 €
Accompanying Person[3)]	25 €

Registrations after March 27, 2013 will be charged a 20 € 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) Participation to the Welcome Reception on May 10, 2013 and the Poster Session on May 11, 2013 are only included.

The conference ticket includes a book of abstracts, a list of participants, meals and beverages during the welcome reception, the poster session and the coffee breaks.

Lunches are not included in the registration fee. Lunch tickets for the KIT Mensa on Friday (May 10) and Saturday (May 11) will cost 12 € each. It is highly recommended to add lunch tickets to your registration, since there are very few opportunities for having lunch nearby the conference venue.

REGISTRATION

Please register online at **www.bunsentagung.de**.

Registration is possible, subject to capacity in the lecture rooms, up to the beginning of the conference. Publication deadline of the list of participants is **April 19, 2013**. It is not guaranteed that registrations received later will appear in the list.

Conference ticket, book of abstracts and list of participants will be handed out on-site.

PAYMENT

Due to organisational constraints we can only accept payment by credit card. You will receive an invoice by mail after your registration has been booked.

CANCELLATION

Only written cancellations will be accepted (letter, fax or e-mail). 30 € administrative costs will be charged for cancellations made before April 19, 2013. 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. Further claims for compensation are excluded.

Special Cancellation Policy for Social Activities:
Conference Dinner: Conference Dinner tickets can be cancelled without charges **before April 5, 2013**. Cancellations received later will not be eligible for any refund.

Guided Walking Tour of Karlsruhe: Tickets for the Guided Walking Tour can be cancelled without charges **before April 19, 2013**. Cancellations received later will not be eligible for any refund.

ACCOMMODATION

You can access a list of hotels with special rates on the conference website **www.bunsentagung.de**, via the item "Accommodation".

Reservations should be directly made to the hotel by the participants. Special rates are subjected to hotel contingent capacity.

If you have any questions or need further information on hotel reservation, please contact directly the Karlsruhe tourism department (Mrs. Stephanie Sivic, Phone: +49 (0)721 3720 5393, E-Mail: stephanie.sivic@karlsruhe-tourismus.de) or check www.karlsruhe-tourismus.de.

VENUE

KIT – Karlsruhe Institute for Technology
Campus South
Fritz-Haber-Weg 2
76131 Karlsruhe

HOW TO REACH THE VENUE

Karlsruhe is easy to travel to. The city has excellent connections to at least 4 airports (Frankfurt, Stuttgart, Strasbourg and Karlsruhe/Baden-Baden) and is quick to reach from the motorway (A5, A61, A8, A5).
Karlsruhe is also a hub for InterCityExpress (ICE), InterCity, EuroCity, InterRegio trains and offers direct connection from Paris with TGV trains.
From the Karlsruhe Railway Station you can reach the KIT-Campus South by tramways (station: "Durlacher Tor/KIT Campus Süd" or "Kronenplatz").

PLEASE NOTE: Construction works could affect the public transport services in Karlsruhe. Regularly updated information on route changes is available at www.kvv.de.

On the conference website www.bunsentagung.de, under the menu "Venue/How to reach the venue", you´ll find detailed driving directions to the KIT-Campus South, as well as information on reduced fare railway tickets to DECHEMA events.

Parking Information: During the Bunsentagung participants can use the parking spaces of the KIT-Campus South (entrance from "Durlacher Tor"), **except on May 10, 2013**. Due to a public holiday in Germany on May 10, 2013 the entrance to KIT-Campus South will be closed. Please use the multistorey car parks "Waldparkplatz" (free of charge - Address: Adenauerring - 76133 Karlsruhe) or "Schlossplatz" (subject to charge - Address: Am Schlossplatz - 76133 Karlsruhe)

OPENING HOURS ON-SITE CONFERENCE OFFICE

Thursday, May 9, 2013	11:00 – 19:00
Friday, May 10, 2013	07:30 – 19:00
Saturday, May 11, 2013	08:00 – 17:00

A separate counter for student travel grants will be open on Friday from 09:00 to 18:00.

CONTACTS

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

Ms Daniela Sabolo
DECHEMA e.V.
Theodor-Heuss-Allee 25
60486 Frankfurt am Main/D
Phone: +49 (0)69 7564-243
Fax: +49 (0)69 7564-176
E-mail: sabolo@dechema.de

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

Mrs Erika Wöhler
Deutsche Bunsen-Gesellschaft für Physikalische Chemie e.V.
German Bunsen Society for Physical Chemistry
Theodor-Heuss-Allee 25
60486 Frankfurt am Main/D
Phone: +49 (0)69 7564-621
Fax: +49 (0)69 7564-622
E-mail: woehler@bunsen.de

CONFERENCE LANGUAGES

The official languages of the conference are English and German.

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 AND POSTER AWARDS

Posters will be on display during the entire conference. There will be a dedicated Poster Session on Friday, May 10, 2013 from 18:00 – 22:00. Authors are asked to be present at their own poster during the Poster Session for discussion.

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 the presentation on the assigned poster board and to remove it at the end of the conference.

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 next Bunsentagung 2014 in Hamburg for the main author. Additionally, another 8 presentations will be selected to receive a "Hot Topic" Poster Award Certificate, which grants free admission to the next Bunsentagung 2014 in Hamburg for the main author.

The Poster Award will take place during the Closing Ceremony on Saturday 11, 2013 at 16:00.

Authors of the selected posters are invited to hold a short presentation of their work (1-2 PowerPoint slides only, best prepared in advance of the conference).

Only authors present at the Closing Ceremony will be awarded.


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KARRIEREFORUM (in German only)

Thursday, May 9, 2013 **11:30 – 14:45** (Room: CRIEGEE)

Topic: **"Anträge, Stipendien, Nachwuchsgruppe – Fördermöglichkeiten für Nachwuchswissenschaftler"**

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

Admission is free, but advance online registration is required. Please tick the appropriate box on the online registration form.

Information material will also be available at the "Karriereforum" stand at the accompanying exhibition.

Jede Wissenschaftlerin und jeder Wissenschaftler ist in ihrem/seinem Berufsleben etliche Male mit dem Schreiben von Projektanträgen beschäftigt. Ob DFG-Einzelantrag, die Finanzierung der eigenen Stelle oder der Nachwuchsgruppe, das Stipendium, der Auslandsaufenthalt oder die Rückkehr aus dem Ausland, immer steht das Verfassen eines Förderantrages oder eines Projektplanes an der ersten Stelle. Wie funktioniert eine solche Antragstellung? Welche Elemente hat ein solcher Projektplan? Welche Formalien und Fristen müssen dabei beachtet werden? Welche Fördermöglichkeiten gibt es überhaupt, speziell zu Anfang der wissenschaftlichen Laufbahn?

Vorläufiges Programm

11:30	**Eröffnung Karriereforum** M. Schnell, Center for Free-Electron Laser Science, Hamburg/D D. Samuelis, Max Planck Institute for Solid State Research, Stuttgart/D
11:45	**Fördermöglichkeiten für Nachwuchswissenschaftler** NN, Deutscher Akademischer Austauschdienst, Bonn/D (angefragt)
12:20	Mittagspause
13:00	**Fördermöglichkeiten für Auslandsaufenthalte und Rückkehr** NN, Alexander-von-Humboldt-Gesellschaft (angefragt)
13:35	**Die DFG informiert – Förderung des wissenschaftlichen Nachwuchses** K. Winkler, Deutsche Forschungsgemeinschaft (DFG), Bonn/D; P. Nürnberger, Universität Würzburg/D
14:00	**Diskussion**
14:30	Ende der Veranstaltung

In der Mittagspause am Freitag, den 10. Mai findet die jährliche Mitgliederversammlung der Arbeitsgemeinschaft Bunsen-Karriereforum statt. Der Ort und die genaue Zeit wird noch bekannt gegeben. Mitglieder und Interessierte sind herzlich zur Teilnahme eingeladen.

LIQUID-CRYSTAL EXHIBITION AT KIT

While attending the Bunsentagung in Karlsruhe, you should not miss the opportunity to visit the permanent liquid-crystal exhibition of the German Bunsen Society. The exhibition is accessible in the ground floor of the building "Flachbau Physik" (Geb: 30.22) in front of "Otto Lehmann-Hörsaal". The exhibition features samples and descriptions of the progress made in the development of liquid crystals and their applications.

CHILD CARE

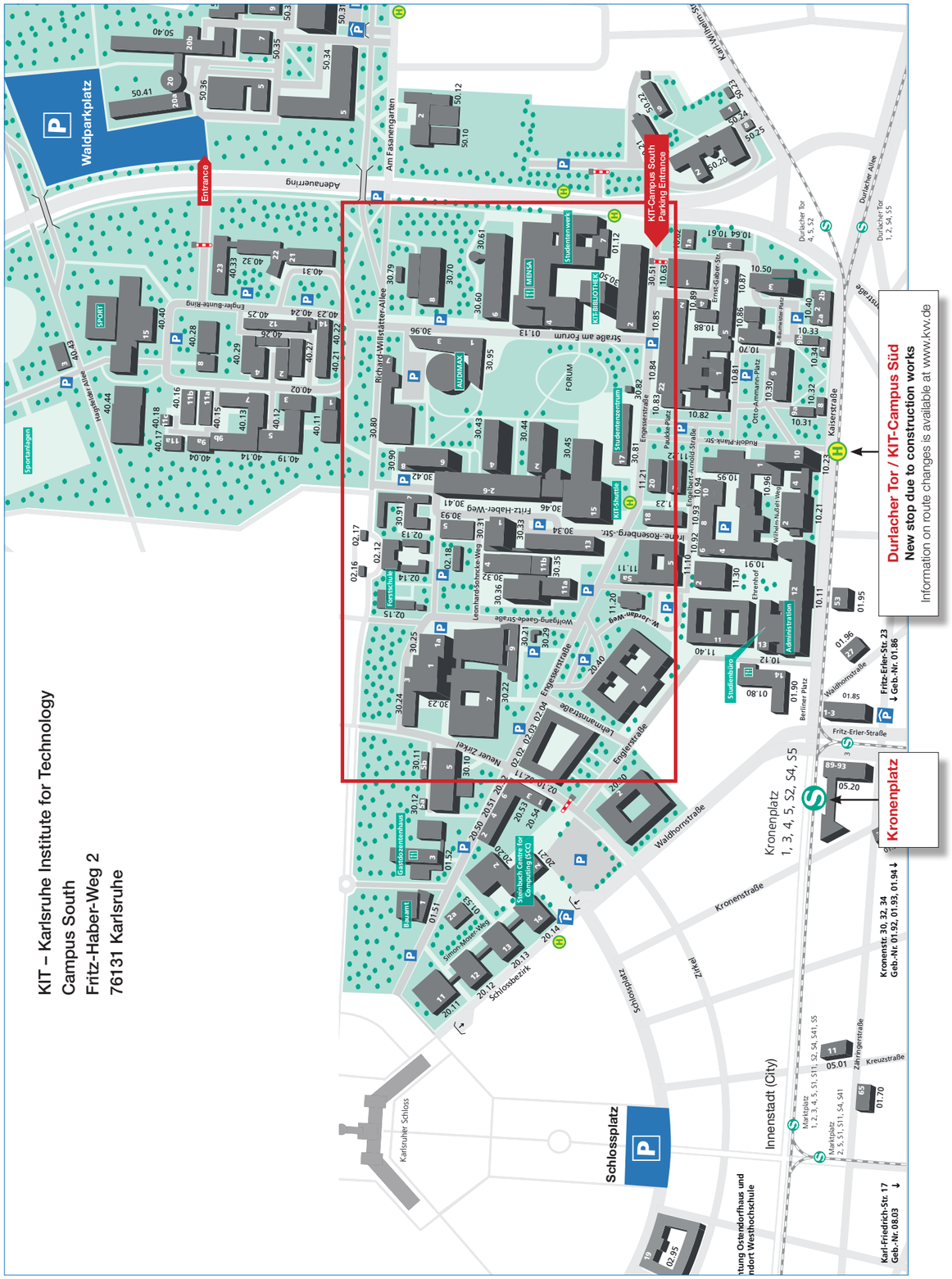
The Bunsentagung offers the opportunity for child care service (subject to extra charge) to parents of small children during the event. Interested parents are requested to contact **Mrs Dagmar Wagner** (bunsen2013@ipc.kit.edu) to discuss their needs.

INTERNET SERVICE

Free internet access via WLAN will be available for all participants during the conference.

More and regularly updated information on the conference is available at

www.bunsentagung.de



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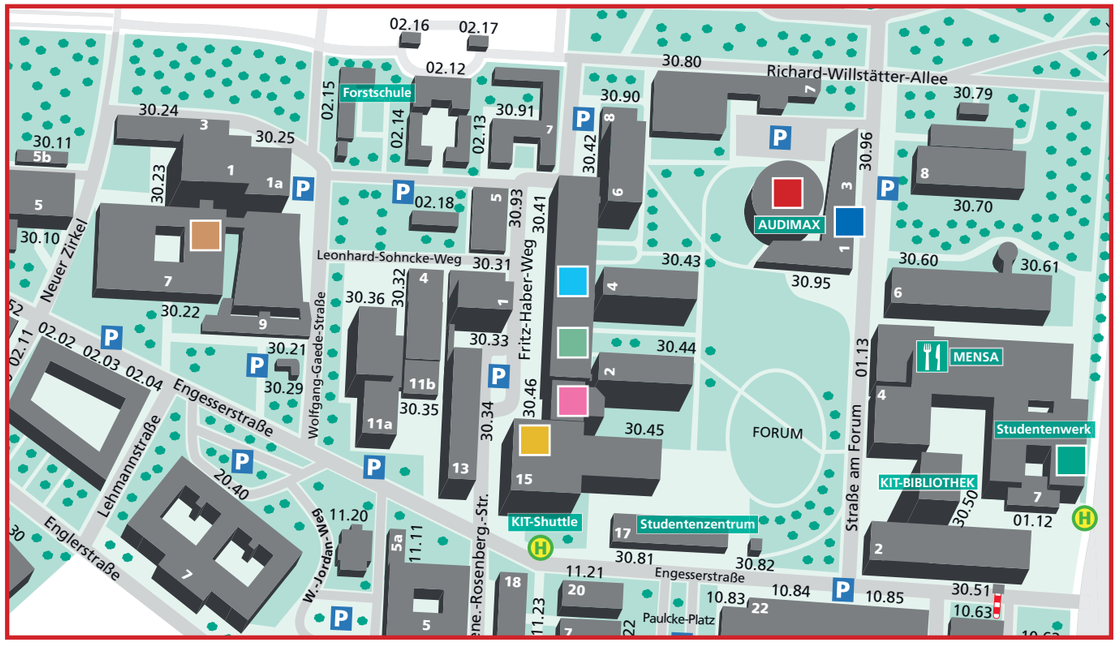
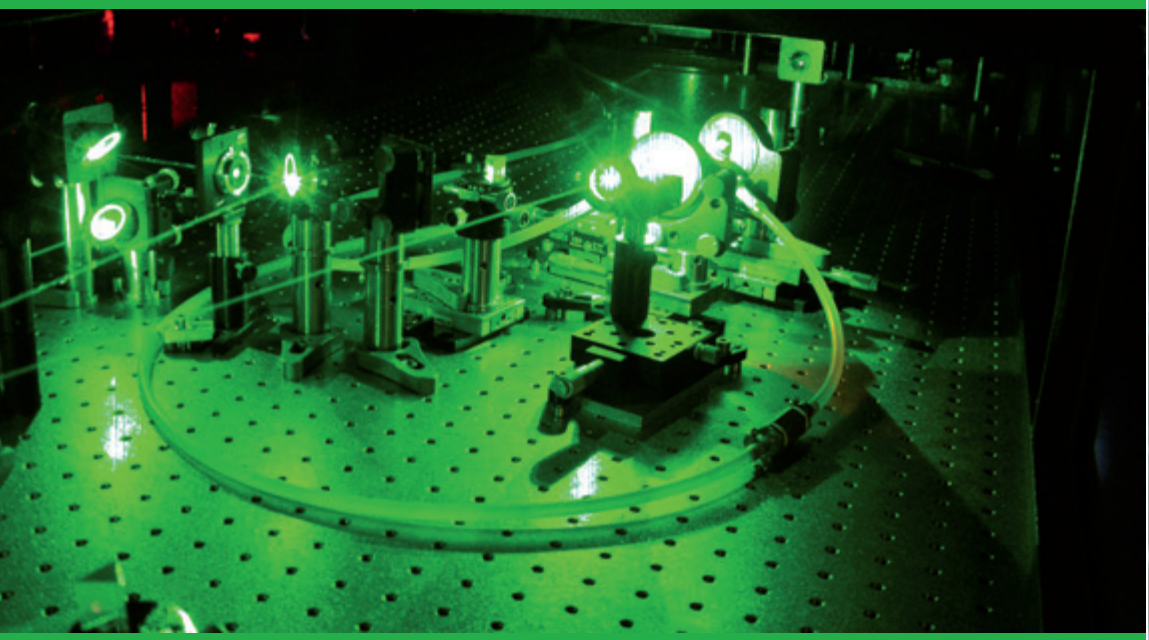
76131 Karlsruhe

- On-site Conference Office / Poster Session (AUDIMAX)
- Lecture Room (AUDIMAX)
- Lecture Rooms (Hörsaal I + II + III, Criegee)
- Lecture Room (Neuer Chemiehörsaal)
- Lecture Room (AOC101)
- Exhibition (Flachbau Chemie)
- Liquid-Crystal Exhibition (Flachbau Physik)
- Welcome Reception (Alte Mensa)
- KIT-Mensa (Lunch)





Deutsche Bunsen-Gesellschaft für Physikalische Chemie e.V.
German Bunsen Society for Physical Chemistry
Theodor-Heuss-Allee 25
60486 Frankfurt am Main/D
Phone: +49 (0)69 7564-621
Fax: +49 (0)69 7564-622
E-Mail: woehler@bunsen.de
Internet: www.bunsen.de

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