

BUNSEN-TAGUNG 2026

Properties and Processes under Confinement

Dresden University of Technology
March 30- April 01, 2026

LECTURE SCHEDULE & POSTER LIST



Deutsche Bunsen-Gesellschaft
für physikalische Chemie

www.bunsentagung.de

BUNSEN-TAGUNG 2026

Properties and Processes under Confinement
Dresden University of Technology, March 30- April 01, 2026
www.bunsentagung.de

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EXHIBITORS

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Exhibition starts at 10:25 on Tuesday & Wednesday

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IMPRINT

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As of March, 24, 2026

16:30 **OPENING CEREMONY** HSZ Hörsaal Audimax

OPENING LECTURE

HSZ Hörsaal Audimax

17:50 **Processing of liquid-phase exfoliated 2D nanomaterials devices**
V. Nicolosi, Dublin/IE

19:00 **Science Dinner**
 Restaurant „Pulverturm an der Frauenkirche“ (registration required)

Tuesday, March 31, 2026, 08:30-09:15

PLENARY LECTURE

HSZ Hörsaal Audimax

08:30 **Self-Assembly of Gold Nanoparticles into Optically Active Nanostructures**
L. M. Liz-Marzán, Donostia-San Sebastian/ES

Tuesday, March 31, 2026, 09:25-10:25

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

09:25 **Some like it cold - from a single-molecule perspective on ice-interactive proteins to chemical cryobiology for improved cryopreservation**
I. Voets, Eindhoven/NL

10:05 **EPR investigations of Molecular Heterogeneous Catalysis in Confined Geometries**
J. Van Slageren, Stuttgart/DE, A. Allgaier, Stuttgart/DE, L. Rautenbach, Stuttgart/DE, R. Peters, Stuttgart/DE

Spectroscopy & Industry Lecture

HSZ Hörsaal 3

09:25 **The recombination dynamics of photoexcited HPTS on a nano- to microsecond timescale**
T. Stensitzki, Potsdam/DE, A. Zehle, Potsdam/DE, H. Müller-Werkmeister, Potsdam/DE

09:45 **Direct Determination of Giant Magnetic Anisotropies in Triplet Main Group Compounds by THz-EPR Spectroscopy**
T. Al Said, Berlin/DE, K. Holldack, Berlin/DE, A. Schnegg, Mülheim a. d. Ruhr/DE

INDUSTRY LECTURE

10:05 **Correlative Photophysical Characterization via Time Resolved and Quantum Yield Method**
N. Danaf, Herrsching a. Ammersee/DE

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal 2

09:25 **Nanostructured diamond for applications in photocatalysis**
A. Krueger, Stuttgart/DE, R. Rodriguez, Stuttgart/DE, R. Rudolf, Stuttgart/DE

09:45 **Small-angle scattering as a versatile tool for the analysis of confined nanostructures**
S. Mascotto, Koblenz/DE

10:05 **The DAGS-Chemistry: Droplet Assisted Growth and Shaping For Synthesis of Polymeric Nano- And Microstructures under Confinement**
S. Seeger, Zurich/CH

Reaction Kinetics and Dynamics

HSZ 401

09:25 **Spectroscopy and dynamics of molecules in highly-excited states**
S. I. Bokarev, Munich/DE

09:45 **Understanding the Enormous Magnetic Field Effects in the flavin photoreceptor protein MagLOV**
R. J. Kutta, Regensburg/DE, N. Archipowa, Regensburg/DE, M. Konheiser, Bayreuth/DE, U. Krauss, Bayreuth/DE

10:05 **Dynamics of CO₂ bond activation by transition metal ions - Competition between spin-changing and spin-conserving pathways**
J. Meyer, Kaiserslautern/DE, M. Meta, Kaiserslautern/DE, Y. Liu, Albuquerque/US, M. E. Huber, Kaiserslautern/DE, M. Wedele, Kaiserslautern/DE, M. Oncak, Innsbruck/AT, H. Guo, Albuquerque/US

09:25-10:25 Panel discussion with Prof. Melanie Schnell (DESY) and Prof. Robert Franke (Ruhr-Universität Bochum)

This interactive panel discussion explores what defines effective leadership in academia and industry, highlighting personal experiences, challenges, and lessons learned from established scientific leaders. The session builds on the leadership focus of the 01/2026 issue of the Bunsen Magazine and provides early career researchers with insights into leadership pathways and responsibilities. The discussion will conclude with an open Q&A, encouraging participants to engage directly with the speakers and reflect on their own leadership development.

Surfaces and Interfaces

HSZ Hörsaal 4

- 09:25 **Control of plasmon-induced molecular dissociation on Au and Ag nanoparticles by molecular surface orientation**
I. Bald, Potsdam/DE, S. Kogikoski Jr., Potsdam/DE, N. Jahn, Potsdam/DE, E. Titov, Potsdam/DE, N. Deepak, Potsdam/DE, O. Henrotte, Potsdam/DE, E. Cortes, Potsdam/DE
- 10:05 **Selective On-Surface Synthesis of Kekulene versus Isokekulene Studied by STM and Orbital Tomography**
S. Wenzel, Marburg/DE, Z. Ruan, Marburg/DE, Q. Fan, Marburg/DE, A. Haags, Jülich/DE, A. Reichmann, Graz/AT, L. Egger, Graz/AT, H. Kirschner, Berlin/DE, T. Naumann, Marburg/DE, S. Werner, Marburg/DE, O. Kleykamp, Marburg/DE, J. Martinez-Castro, Jülich/DE, F. Lüpke, Jülich/DE, F. C. Bocquet, Jülich/DE, C. Kumpf, Jülich/DE, S. Soubatch, Jülich/DE, A. Gottwald, Berlin/DE, G. Koller, Jülich/DE, M. G. Ramsey, Graz/AT, M. Richter, Berlin/DE, J. Sundermeyer, Marburg/DE, P. Puschnig, Graz/AT, J. M. Gottfried, Marburg/DE, F. S. Tautz, Jülich/DE

Tuesday, March 31, 2026, 10:25 - 11:00

10:25 **COFFEE BREAK**

EXHIBITION OPEN

HSZ / all floors

Tuesday, March 31, 2026, 11:00-12:00

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

- 11:00 **Lighting Up the Force: Remote Sensing of Mechanical Forces via Photon Avalanche under Nanoscale Confinement**
N. Fardian-Melamed, New York/US
- 11:40 **Red-to-blue photon upconversion nanoparticles catalyze radical polymerizations in water**
D. Hübner, Osnabrück/DE, C. Le, Mulhouse/FR, A. Spangenberg, Mulhouse/FR, P. Jin, Konstanz/DE, C. Wang, Konstanz/DE

Spectroscopy

HSZ Hörsaal 3

- 11:00 **Two-Dimensional Infrared Spectroscopy of the SURMOF Cu(Da-DBDC)**
C. Gräve, Bonn/DE, A. C. Fingolo, Karlsruhe/DE, J. Brückel, Karlsruhe/DE, L. I. Domenianni, Bonn/DE, J. Lindner, Bonn/DE, S. Bräse, Karlsruhe/DE, C. Wöll, Karlsruhe/DE, P. Vöhringer, Bonn/DE
- 11:20 **Chiroptical amplification beyond enantiopurity**
A. Kartouzian, Garching/DE, Ch. Panagiotopoulou, Garching/DE, S. Liu, Heidelberg/DE, J. Pittrich, Garching/DE, M. Ganahl, Garching/DE, H. Iglev, Garching/DE, F. Deschler, Heidelberg/DE
- 11:40 **Structure–Dynamics–Function Relationships in Carbon Nitride Photocatalysts: From Ionic PHIs to Nitrogen-Rich g-C₃N₂ Heterojunctions**
A. Konar, Jena/DE, J. Liessem, Ulm/DE, P. Saini, Jena/DE, J. Griebel, Leipzig/DE, R. Beranek, Ulm/DE, B. Dietzek-Ivanšić, Leipzig/DE

2D Materials

HSZ Hörsaal 2

- 11:00 **Next Generation 2D Materials and Their Heterostructures**
R. Friedrich, Dresden/DE, T. Barnowsky, Dresden/DE, A. Nihei, Dresden/DE
- 11:40 **Influence of sub-nanometer porosity on the permeation mechanisms of 1 nm thick molecular carbon nanomembranes**
D. Hüger, Jena/DE, A.-L. Gaus, Ulm/DE, V. Müller, Jena/DE, J. Picker, Jena/DE, M. Frey, Jena/DE, C. Neumann, Jena/DE, M. von Delius, Ulm/DE, A. Turchanin, Jena/DE

TUESDAY MORNING Parallel Sessions 2 // 11:00-12:00

Reaction Kinetics and Dynamics

HSZ 401

- 11:00 **Does charge matter in condensed gas phase chemistry? Achievements, challenges and perspectives**
G. Niedner-Schatteburg, Kaiserslautern/DE, N. Wolfgramm, Kaiserslautern/DE, C. van Wüllen, Kaiserslautern/DE
- 11:20 **Mechanistic Insights into Fe²⁺ Formation in FeCl₃/TRITON X-100 Systems via Pulse Radiolysis**
A. Kahnt, Leipzig/DE
- 11:40 **Steric Shielding Effects on the Kinetics of MR-TADF Emitters**
K. M. Knötig, Siegen/DE, T. Lenzer, Siegen/DE, K. Oum, Siegen/DE

yPC-Session "Meet the young Physical Chemists"

HSZ 403

11:00-11:30 This session offers participants the opportunity to meet members of the yPC core team and learn more about the initiative's activities and opportunities. Attendees can ask questions about yPC programmes, networking opportunities, and ways to become involved in shaping the early career community within the Bunsen-Gesellschaft. The informal format encourages open exchange and provides a platform for participants to connect directly with the yPC team.

Catalysis

HSZ Hörsaal 4

- 11:00 **Photocatalytic Activity of Ion-Exchanged in Poly(heptazine imide) Materials Using First-Principles Many-Body Perturbation Theory**
Z. Hajjahmadi, Görlitz/DE, T. D. Kühne, Görlitz/DE
- 11:20 **Investigating the role of water in low temperature CO₂ reduction at defective TiO₂ using operando-XPS**
J. Klimek, Oldenburg/DE, F. Hallböök, Lund/SE, N. Kruse, Oldenburg/DE, F. Li, Oldenburg/DE, S. Blomberg, Lund/SE, K. Al-Shamery, Oldenburg/DE, L. Mohrhusen, Oldenburg/DE
- 11:40 **Computational Analysis of Divergent HAT Pathways in Pyrimidopteridinetetraone Photocatalysis**
O. S. Bokareva, Rostock/DE, Z. Amanollahi, Rostock/DE, T. Taeufer, Rostock/DE, J. Pospech, Rostock/DE, L. Zach, Rostock/DE, T. H. Vuong, Rostock/DE, O. S. Bokareva, Leibniz/DE

Tuesday, March 31, 2026, 12:00-13:15

12:00-13:15

LUNCH

EXHIBITION OPEN

HSZ / all floors

Tuesday, March 31, 2026, 13:15-14:15

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

- 13:15 **Behavior of Water Confined in Zeolites: Effects of Framework, Si/Al Ratio, and Water Loading from a New General ML Potential**
F. Berger, Cambridge/GB, A. Ramanaviciute, Cambridge/GB, H. Rauch, Cambridge/GB, M. Wang, Cambridge/GB, C. Schran, Cambridge/GB
- 13:35 **Tailor-made mesoporous support materials for catalysis in confinement on the example of the CO₂ hydrogenation reaction**
J. R. Bruckner, Stuttgart/DE, S. Itzigebl, Stuttgart/DE, W. Barakat, Stuttgart/DE, T. Ott, Stuttgart/DE, M. Benz, Stuttgart/DE, D. P. Estes, Stuttgart/DE
- 13:55 **Atomistic Insights into Confined Water Diffusion in MOF-303**
V. Karpov, Berlin/DE, J. Sauer, Berlin/DE, F. Berger, Berlin/DE

Spectroscopy

HSZ Hörsaal 3

- 13:15 **Spectroscopy of Astrophysically Relevant Molecules: Could Some Diffuse Interstellar Bands Belong to Iron Complexes?**
M. Oncak, Innsbruck/AT, S. Jin, Innsbruck/AT, C. van der Linde, Innsbruck/AT, M. Juanes, Valladolid/ES, N. Przybilla, Innsbruck/AT, M. K. Beyer, Innsbruck/AT
- 13:35 **Probing the Fluorescence of Single Quantum Dots in the Gas Phase**
K. Papagrigoriou, Leipzig/DE, F. Funk, Hamburg/DE, S. Zeller, Hamburg/DE, K. R. Asmis, Leipzig/DE, A. Mews, Hamburg/DE, B. Bastian, Leipzig/DE
- 13:55 **Temperature- and matrix-dependent excited state properties in pyrene-linked ruthenium(II) complexes**
K. Rediger, Kaiserslautern/DE, A. C. Sell, Mainz/DE, C. Kerzig, Mainz/DE, M. Wächtler, Kiel/DE

2D Materials

HSZ Hörsaal 2

- 13:15 **Interactions of Molecules with 2D materials: a Driving Force for Modulation of Electronic Properties**
B. Paulus, Berlin/DE
- 13:35 **Colloidal synthesis of 2D klockmannite copper selenide nanocrystals and their photo-physical properties**
U. Parekh, Rostock/DE, S. Dabelstein, Rostock/DE, J. Kaushal, Rostock/DE, R. Lesyuk, Rostock/DE, C. Klinke, Rostock/DE
- 13:55 **Redox-Driven Structural Reorganisation in a 2D conjugated MOF**
F. Reichmayr, Dresden/DE, G. Zhang, Hongkong/HK, I. M. Weidinger, Dresden/DE

Reaction Kinetics and Dynamics

HSZ 401

- 13:15 **Rethinking of the determination of activation energies in solution**
S. Landgraf, Graz/AT, P. Choto, Chinag Rai/TH
- 13:35 **Impact of Hydration on the Reactivity of Peroxycarbonate Radical Anions with Formic Acid**
C. van der Linde, Innsbruck/AT, D. Jank, Innsbruck/AT, C. H. Ng, Kuala Lumpur/MY, M. K. Beyer, Innsbruck/AT, W. K. Tang, Kuala Lumpur/MY
- 13:55 **Kinetic Experiments in Ion Traps under Multicollisional Conditions**
J. Lengyel, Garching/DE, K. Li, Garching/DE, Y. Yan, Garching/DE

yPC Career Forum + World Café with Industry

HSZ 403

13:15-14:15 The yPC Career Forum and World Café connects early career researchers with industry representatives in an interactive and informal networking format. Participants will rotate between small discussion tables hosted by industry professionals, enabling direct conversations about career paths, required skills, and opportunities beyond academia. This session aims to facilitate meaningful exchange, provide career orientation, and strengthen connections between young scientists and industrial partners.

Biophysical Chemistry & Catalysis

HSZ Hörsaal 4

- 13:15 **Structural Dynamics as Window into Biological Function**
H. Müller-Werkmeister, Potsdam/DE
- 13:55 **Nanostructured photoelectrodes for photoelectrochemical water splitting**
R. Marschall, Bayreuth/DE

Tuesday, March 31, 2026, 14:15-14:40

14:15

COFFEE BREAK

EXHIBITION OPEN

HSZ / all floors

Tuesday, March 31, 2026, 14:40-16:00

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

- 14:40 **Electron transfer networks under protein confinement: aromatic Tyr/Trp pathways modulate ROS formation in multicopper oxidase**
P. Kielb, Bonn/DE, C. Scharbach, Bonn/DE, F. H. Pilz, Bonn/DE
- 15:00 **Directing the mobility of guest molecules under nanoporous confinement by linearly polarized light**
T. Al Najjar, Berlin/DE, C. Li, Karlsruhe/DE, Y. Jiang, Karlsruhe/DE, L. Heinke, Berlin/DE
- 15:20 **Molecular Orientation Effects on SERS Spectra at the Single-Molecule Level Revealed by DNA Origami Plasmonic Antennas**
S. Kogikoski Jr, Potsdam/DE, Y. Kanehira, Potsdam/DE, E. Titov, Potsdam/DE, P. Saalfrank, Potsdam/DE, A. K. Adamczyk, Fribourg/CH, K. Kolataj, Fribourg/CH, G. P. Acuña, Fribourg/CH, I. Bald, Potsdam/DE
- 15:40 **Tunable Multiexciton Properties of Colloidal Quantum Dots**
R. Baruah, Kiel/DE, K. Kumar, Oldenburg/DE, M. Wächtler, Kiel/DE

Spectroscopy

HSZ Hörsaal 3

- 14:40 **Time-Resolved Quantum Cascade Laser Infrared Spectroscopy: Unraveling the Photoreduction Mechanism of Cryptochrome**
M. M. Diedrich, Bielefeld/DE, E. Coman, Bielefeld/DE, L. Gött-Zink, Bielefeld/DE, T. Kottke, Bielefeld/DE

- 15:00 **Investigation of Chiral Copolymer Thin Films on Photoalignment Layers using Müller Matrix and Transient CD Spectroscopy**
D. Gust, Siegen/DE, V. Schumacher, Siegen/DE, N. Schmidt, Siegen/DE, K. Oum, Siegen/DE, T. Lenzer, Siegen/DE
- 15:20 **Excitation-wavelength dependent dynamics of [Ge₉] clusters: lifetime tuning and solvated electrons**
M. Jänchen, Garching/DE, A. Fischbacher, Garching/DE, E. Thyraug, Garching/DE, T. Fässler, Garching/DE, J. Hauer, Garching/DE
- 15:40 **The universal vibrational dynamics of water bound to tertiary amines: more than just Fermi resonance**
E. Lwin, Göttingen/DE, N. O. B. Lüttschwager, Göttingen/DE, M. A. Suhm, Göttingen/DE

DBG Award Winners

HSZ Hörsaal 2

- 14:40 **Ewald-Wicke-Preis**
NIR-Fluorescent Materials for Biomedical Imaging and Sensing
R. Nißler, Zürich/CH
- 15:00 **Nernst-Haber-Bodenstein-Preis**
Optics of single molecules explored with sub-nm precision
A. Rosławska, Stuttgart/DE
- 15:20 **van 't Hoff-Preis**
Intermolecular interactions revealed with rotational spectroscopy: Structure, dynamics, and chirality
M. Schnell, Kiel/DE
- 15:40 **DBG-Ehrenmitgliedschaft**
Fuel, Fire, Future: Combustion Beyond the Fossil Era
K. Kohse-Höinghaus, Bielefeld/DE

Biophysical Chemistry and Biophotonics

HSZ 401

- 14:40 **Exploring Biomolecular Interactions, Molecular Dynamics Force Fields and Nanoconfinement Using Vibrational Stark Probes**
J. Kozuch, Berlin/DE
- 15:20 **Multidimensional ultrafast fluorescence spectroscopy: the keto-carotenoid peridinin as a test case**
J. Hauer, Garching/DE, H. Hao, Garching/DE
- 15:40 **Redox tuning of engineered heme protein active sites and catalytic implications**
M. Mahler, Bonn/DE, P. Kielb, Bonn/DE

Energy Storage

HSZ 403

- 14:40 **In-situ IR Spectroscopy of N-Methylphthalimide for Organic Redox Flow Batteries: Mechanisms and Decomposition Pathways**
G. Rossetto, Erlangen/DE, D. Schaueremann, Erlangen/DE, E. Franz, Erlangen/DE, J. Steffen, Erlangen/DE, A. Görling, Erlangen/DE, R. Marrazzo, Novara/IT, S. Leonardi, Novara/IT, O. Brummel, Erlangen/DE, J. Libuda, Erlangen/DE
- 15:00 **Investigating Water-Modified Solvate Ionic Liquids: Molecular Insights into Lithium Solvation and Transport**
J. K. Philipp, Rostock/DE, D. Paschek, Rostock/DE, R. Ludwig, Rostock/DE
- 15:20 **Understanding the Performance Enhancing Effects of Pulsed Current Charging for Lithium- vs. Sodium-Ion Batteries**
W. Schwedland, Berlin/DE, P. Adelhelm, Berlin/DE
- 15:40 **Energy Landscapes and Structure in Ion Conducting Solids – DFG Research Unit FOR_5065**
K.-M. Weitzel, Marburg/DE

Surfaces and Interfaces

HSZ Hörsaal 4

- 14:40 **Leveraging Conformationally-Fluorescent Polymers for In Situ Sensing of Physicochemical Phenomena**
Q. A. Besford, Dresden/DE
- 15:20 **Solvent Composition and Structure near Amphiphilic Solutes in Three-Component Aqueous Mixtures**
E. Casalini, Duisburg/DE, A. M. Stingel, Bochum/DE, B. Moussa, Bochum/DE, M. Personeni, Bochum/DE, P. B. Petersen, Bochum/DE, A. Vila Verde, Duisburg/DE
- 15:40 **Carbon Impurity Entrapping and Charge Localization within TiO₂ Nanoparticle Films**
G. Vives Ollé, Salzburg/AT, T. Berger, Salzburg/AT, G. Bourret, Salzburg/AT, O. Diwald, Salzburg/AT

Tuesday, March 31, 2026, 16:15-18:45

16:15-17:30 POSTER SESSION PART I -- EVEN NUMBERS

17:30-18:45 POSTER SESSION PART II -- ODD NUMBERS



PLENARY LECTURE

HSZ Hörsaal Audimax

08:30 **Local thermodynamics and electric fields at an electrified interface**
M. Havenith, Bochum/DE

Wednesday, April 01, 2026, 09:25-10:25

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

09:25 **Nanoconfinement Materials as a Platform to Investigate Charge Storage Properties at Confined Electrochemical Interfaces**
S. Fleischmann, Ulm/DE

10:05 **Charge Carrier Dynamics in Strongly Confined Transition Metal Dichalcogenides in Colloidal Solution**
M. Fröhlich, Tübingen/DE, S. Kumar, Jena/DE, T. Braun, Tübingen/DE, M. Kögel, Reutlingen/DE, C. Cocchi, Jena/DE, J. C. Meyer, Tübingen/DE, J. Lauth, Tübingen/DE

Spectroscopy

HSZ Hörsaal 3

09:25 **Influence of the Bridging Length on the Ultrafast Isomerization Dynamics of Bridged Azobenzenes in a Molecular Beam**
P. Pessier, Freiburg/DE, M. Hergert, Kiel/DE, L. Guhl, Kiel/DE, F. Temps, Kiel/DE

09:45 **Formation of HNC and HCN isomers in molecular plasmas revealed by frequency comb and quantum cascade laser spectroscopy**
I. Sadiq, Bochum/DE, S. Di Bernardo, Caserta/IT, U. Macherius, Greifswald/DE, J. H. van Helden, Bochum /DE

10:05 **THz Pump Pulse Drives Nonlinear H-bond Dynamics in Liquid Water**
P. Schienbein, Bochum/DE

Electrochemistry

HSZ Hörsaal 2

09:25 **Liquid-metal GaInSn-based electrocatalysts for the reduction of CO₂ to solid carbon: Improved understanding from experiment and modelling**
M. M. May, Tübingen/DE, D. Lörch, Tübingen/DE, M. Übele, Tübingen/DE, A. G. A. Mohamed, Tübingen/DE, H. Euchner, Tübingen/DE, P. Bogdanoff, Berlin/DE

09:45 **Electroreduction of Acetone on PtRu Model Catalysts**
O. Brummel, Erlangen/DE, J. Libuda, Erlangen/DE, R. Hübsch, Erlangen/DE, D. Schauermaier, Erlangen/DE, P. K. Samal, Prague/CZ, J. Škvára, Prague/CZ, F. Jäschke, Erlangen/DE, L. Piliš, Prague/CZ, T. Skála, Prague/CZ, N. Tsud, Prague/CZ, J. Mysliveček, Prague/CZ, Y. Lykhach, Erlangen/DE

KEY TOPIC: Properties and Processes under Confinement

HSZ 401

09:25 **Confinement of chemical moieties in evaporating droplets: spray-drying as a forced assembly technique to pave the way to highly functional materials**
K. Mandel, Erlangen/DE

09:45 **Fe(III) Complex-Sensitized Photon Upconversion Nanoparticles for Photocatalysis**
C. Wang, Konstanz/DE

10:05 **Liquid or ice? The structure of water in nanoporous environments**
E. von Domaros, Jena/DE, M. A. Nadeem, Jena/DE

Theory and Data Science

HSZ 403

09:25 **Generative Path Integral Monte Carlo Sampling**
Z. Aigner, Innsbruck/AT, M. Ončák, Innsbruck/AT, M. Hütter, Innsbruck/AT

09:45 **Linear-scaling DLPNO-MP2 for periodic systems**
A. Nejad, Oxford/GB, A. Zhu, Oxford/GB, K. Sorathia, Oxford/GB, D. Tew, Oxford/GB

10:05 **Accurate continuum solvation for fast modern semiempirical electronic**
R. Dahl, Bonn/DE, T. Froitzheim, Bonn/DE, L. Wittmann, Bonn/DE, S. Grimme, Bonn/DE

PCCP Prize Lecture & DFG Lecture

HSZ Hörsaal 4

09:25 **PCCP Emerging Investigator**
Computational Surface Models for Oxygen Evolution Reaction
K. S. Exner, Essen/DE

10:05 **DFG-Lecture**
Deutsche Forschungsgemeinschaft (DFG): Funding Opportunities for Early Career Researchers at a Glance
W. Wachter, Bonn/DE

10:25

COFFEE BREAK



Wednesday, April 01, 2026, 11:00-12:20

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

- 11:00 **SAXS/WAXS Study of Covalently Linked CdSe and CdS Magic-size Cluster Chains**
K. Boldt, Rostock/DE, A. Cedrowicz, Rostock/DE, T. H. Luong, Rostock/DE, P. Schwarz, Leoben/AT, S. Haas, Hamburg/DE, R. T. Lechner, Leoben/AT
- 11:20 **Optically Active Plasmonic Nanostructures via Colloidal Self-Assembly and Light-Directed Growth**
Y. Cai, Dresden/DE, C. Rossner, Dresden/DE, N. A. Kotov, Ann Arbor/US
- 11:40 **Small-Angle Scattering Analysis of Catalyst-Supporting Ionic Liquid Films in Ordered Mesoporous Silica**
J. Fischer, Stuttgart/DE, N. Schnabel, Stuttgart/DE, H. B. Duc, Stuttgart/DE, B. Atwi, Stuttgart/DE, J. Bruckner, Stuttgart/DE, Y. Liu, Gaithersburg/US, M. R. Buchmeiser, Stuttgart/DE, T. Sottmann, Stuttgart/DE
- 12:00 **Small-angle scattering insights into the equilibrium or metastable nature of capillary condensation**
C. Gommès, Liege/BE, A. F. Haidar, Liege/BE, A. Belet, Liege/BE, B. Goderis, Leuven/BE, A. Léonard, Liege/BE

Spectroscopy

HSZ Hörsaal 3

- 11:00 **Beyond isotropic reorientation: Probing anisotropic and internal motions in ionic liquids**
A. Strate, Rostock/DE, L. Kruse, Rostock/DE, D. Paschek, Rostock/DE, R. Ludwig, Rostock/DE
- 11:20 **Tracking Ultrafast Energy and Electron Transfer in Cu(I)-BODIPY Bichromophores**
M. K.-E. Wolff, Braunschweig/DE, K. J. Haseloff, Braunschweig/DE, R. Frank, Braunschweig/DE, S. Tschierlei, Braunschweig/DE, M. Karnahl, Braunschweig/DE
- 11:40 **Ligand effects on the photoluminescence-spectroelectrochemical response of CdS-based nanostructures**
J. Voß, Hamburg/DE, C. Strelow, Hamburg/DE, T. Kipp, Hamburg/DE, A. Mews, Hamburg/DE
- 12:00 **THz Calorimetry of Aqueous Electrolyte Solutions**
G. Schwaab, Bochum/DE, C.-Y. Ma, Braunschweig/DE, S. Pezzotti, Paris/FR, M. Havenith, Bochum/DE

Electrochemistry

HSZ Hörsaal 2

- 11:00 **Electrochemical Concepts for Understanding Dynamic Electrocatalyst Interfaces: Insights from Impedance Spectroscopy and Structural Operando Methods**
J. Linnemann, Paderborn/DE
- 11:40 **Electrochemically generated cementitious precursors towards sustainable cement production**
A. Ramuglia, Dresden/DE, P. Ly, Dresden/DE, V. Bon, Dresden/DE, J. Scheel, Dresden/DE, T. Köberle, Dresden/DE, V. Mechtcherine, Dresden/DE, M. Liebscher, Dresden/DE, I. Weidinger, Dresden/DE
- 12:00 **Ion and Water Dynamics under Confinement in Transition Metal Oxide Electrodes Probed by Dual-Modality Fast EQCM-D and Raman Spectroscopy**
C. Leppin, Paderborn/DE, R. Shashindra, Paderborn/DE, O. Röth, Paderborn/DE, J. Linnemann, Paderborn/DE

Biophysical Chemistry and Biophotonics

HSZ 401

- 11:00 **Competitive Adsorption of a Monoclonal Antibody and Amphiphilic Surfactants to the Air-Water Interface**
C. Schwieger, Halle (Saale)/DE, P. Garidel, Biberach/DE, M. Blech, Biberach/DE, E. Hingst, Halle (Saale)/DE, D. Hinderberger, Halle (Saale)/DE
- 11:20 **Influence of α -Helical Content on the Thermodiffusion of Apomyoglobin**
S. Wiegand, Jülich/DE, B. A. Rudani, Jülich/DE, S. Docter, Jülich/DE, S. Schott-Verdugo, Jülich/DE, J. Buitenhuis, Jülich/DE, H. Gohlke, Jülich/DE, A. M. Stadler, Jülich/DE
- 11:40 **UV Resonance Raman Spectroscopic Marker Bands of Base Pair Formation During Nucleic Acids Assembly**
A.-S. Schüen, Bonn/DE, B. Bädorf, Bonn/DE, A. Bumberger, Bonn/DE, D. Kendirlik, Bonn/DE, S. Kath-Schorr, Bonn/DE, S. Grimme, Bonn/DE, P. Kielb, Bonn/DE
- 12:00 **Insights into the Mechanism of a Human ABC Transporter by Perfusion-Induced ATR FTIR Difference Spectroscopy**
C. Strothenke, Bielefeld/DE, H. Bockhorn, Bielefeld/DE, T. Kottke, Bielefeld/DE

- 11:00 **Confinement-Guided Nanoscale Electropolymerization of Melanin with Scanning Electrochemical Cell Microscopy (SECCM)**
N. Al-Shamery, Coventry/GB, D. Valavanis, Coventry/GB, P. S. Lee, Singapore/SG, P. R. Unwin, Coventry/GB
- 11:20 **Chiral Control of Gas-Phase Molecules using Microwave Pulses**
F. E. L. Berggötz, Hamburg/DE, M. Leibscher, Berlin/DE, W. Sun, Hamburg/DE, H. Singh, Garching/DE, C. P. Koch, Berlin/DE, M. Schnell, Hamburg/DE
- 11:40 **Advancement in Metal Aerogels: From Porous Thin Films to Two-Dimensional Materials**
P. Khavlyuk, Bochum/DE
- 12:00 **Nuclear dimensions for electron transfer in mixed-valent systems**
A. Šrut, Darmstadt/DE, B. J. Lear, State College/US, V. Krewald, Darmstadt/DE

Surfaces and Interfaces

HSZ Hörsaal 4

- 11:00 **Efficient quantum defect incorporation into fluorescent carbon nanotubes**
V. D. Andreeva, Bochum/DE, J. T. Metternich, Bochum/DE, C. Ma, Bochum/DE, J. A. C. Wartmann, Bochum/DE, S. Kruss, Bochum/DE
- 11:20 **Interfacial Adhesion Mechanisms of Mucins Studied by Atomic Force Microscopy**
B. N. Balzer, Freiburg/DE
- 11:40 **Nanoscale Dynamics in Confined Microemulsions**
S. Wellert, Berlin/DE, M. Dahl, Berlin/DE, I. Hofmann, Grenoble/FR, O. Holderer, Garching/DE, T. Hellweg, Bielefeld/DE
- 12:00 **Photoactivated Titania Nanocrystal Thin Film Chemiresistors**
F. Dobschall, Hamburg/DE, S. C. Bittinger, Donostia-San Sebastian/ES, T. Vossmeier, Hamburg/DE

Wednesday, April 01, 2026, 12:20-13:30

12:25-13:30 LUNCH



Wednesday, April 01, 2026, 13:30-14:15

PLENARY LECTURE

HSZ Hörsaal Audimax

- 13:30 **Confinement Effects in Porous Carbon-based Materials and their impact in Catalysis and Electrochemical Energy Storage**
M. Oschatz, Jena/DE

Wednesday, April 01, 2026, 14:25-15:25

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal Audimax

- 14:25 **Leveraging molecular simulations to corroborate confinement effects observed in mesoporous materials**
N. Hansen, Stuttgart/DE, M. Högler, Stuttgart/DE, H. Kraus, Stuttgart/DE
- 14:45 **Photocharging in Plasmon-Driven Catalysis**
W. Koopman, Potsdam/DE, F. Stete, Potsdam/DE, K. Peikert, Potsdam/DE, M. Bargheer, Potsdam/DE

KEY TOPIC: Properties and Processes under Confinement

HSZ Hörsaal 3

- 14:25 **Mechanism and Dynamics of Urea Macrocyclization under Cavitand Confinement in Aqueous Solution**
L. Araujo, Bochum/DE, G. Tusha, Bochum/DE, L. Schäfer, Bochum/DE
- 14:45 **Observation of ultrafast sub-diffusion of a molecule in a nanoparticle**
L. Bruder, Freiburg/DE, A. Morlok, Freiburg/DE, Y. Li, Freiburg/DE, U. Bangert, Freiburg/DE, F. Riedel, Freiburg/DE, F. Stienkemeier, Freiburg/DE
- 15:05 **Infrared Spectroscopy on Light Receptors in Living Human Cells**
L. Gött-Zink, Bielefeld/DE, C. Mann, Bielefeld/DE, K. M. Müller, Bielefeld/DE, T. Kottke, Bielefeld/DE

Electrochemistry

HSZ Hörsaal 2

- 14:25 **Electrochemical Recovery of Carbon Fibers from Carbon Fiber Reinforced Concrete using Environmentally Friendly Electrolytes**
S. Röher, Dresden/DE, J. Scheel, Dresden/DE, A. Apel, Dresden/DE, M. Liebscher, Dresden/DE, I. M. Weidinger, Dresden/DE
- 14:45 **Bipolar Electrochemistry in Microfluidic Devices**
F. Kühling, Oldenburg/DE, G. Wittstock, Oldenburg/DE
- 15:05 **High-Resolution Electrochemical 3D Printing Enabled by Nanoscale Confinement**
D. Momotenko, Oldenburg/DE, K. A. Kanes, Oldenburg/DE, J. Mead, Oldenburg/DE, P. Zeng, Zürich/CH, M. Claussen, Oldenburg/DE, S. Fatikow, Oldenburg/DE

Biophysical Chemistry and Biophotonics

HSZ 401

- 14:25 **Near infrared imaging of hydrogen peroxide mediated stress in plants**
L. Jiaqi, Bochum/DE, S. Kruss, Bochum/DE
- 14:45 **Lipid Scrambling by SND3 in the SEC61 Translocon Complex**
S. Mukherjee, Frankfurt am Main/DE, T. J. Yang, Frankfurt am Main/DE, J. D. Langer, Frankfurt am Main/DE, G. Hummer, Frankfurt am Main/DE, M. A. McDowell, Frankfurt am Main/DE
- 15:05 **Revisiting the activation mechanism of Drosophila melanogaster Cryptochrome**
N. Archipowa, Regensburg/DE, R. J. Kutta, Regensburg/DE

Theory and Data Science

HSZ 403

- 14:25 **A Bottom-Up Approach: Predicting Frequency-dependent NMR Relaxation Rates for “Water-in-Salt” Electrolytes**
A. M. Chiramel Tony, Rostock/DE, L. Kruse, Rostock/DE, A. Strate, Rostock/DE, K. Kamau, Olsztyn/PL, D. Kruk, Olsztyn/PL, R. Ludwig, Rostock/DE, D. Paschek, Rostock/DE
- 14:45 **Intermolecular potentials of π -stacked aggregates are reflecting the oscillations of electronic wavefunctions**
R. F. Fink, Tübingen/DE
- 15:05 **Efficient uLAST/LAST implementations for JW-transformed spin Hamiltonians**
S. Ghassemi Tabrizi, Dresden/DE

Catalysis

HSZ Hörsaal 4

- 14:25 **Activation of atomically precise monolayer-protected Pt nanoclusters: Formation of active CO oxidation catalysts**
P. Chakraborty, Karlsruhe/DE, M. Neumaier, Karlsruhe/DE, J. Seibel, Karlsruhe/DE, N. D. Roit, Karlsruhe/DE, A. Böttcher, Karlsruhe/DE, C. Schmitt, Karlsruhe/DE, D. Wang, Karlsruhe/DE, C. Kübel, Karlsruhe/DE, S. Behrens, Karlsruhe/DE, M. M. Kappes, Karlsruhe/DE
- 14:45 **Controlling and Catalysis of the Formation of Silver Nanocubes in Nonpolar Solvents**
C. Graf, Darmstadt/DE, M. Joschko, Darmstadt/DE, M. Schattmann, Darmstadt/DE, D. Grollmusz, Darmstadt/DE, T. Reich, Mainz/DE
- 15:05 **Cobalt-Doped Lanthanum Aluminate as a Catalyst for Higher Alcohol Synthesis**
H. Stoffel, Koblenz/DE, E. Remark, Koblenz/DE, S. Mascotto, Koblenz/DE, A. Latsiou, Kozani/GR, N. Charisiou, Kozani/GR, M. Goula, Kozani/GR

Wednesday, April 01, 2026, 15:40 - 16:15

15:40 **Poster Awards and Closing Session**

HSZ Hörsaal Audimax

KEY TOPIC 01: Properties and Processes under Confinement

P01_01	<p>Characterizing Ultrafast Processes in Colloidal Transition Metal Diselenides by Transient Absorption and Potential Modulated Absorption Spectroscopy <u>O. Strolka, Tübingen/DE</u>, S. Westendorf, Tübingen/DE, M. Fröhlich, Tübingen/DE, D. A. Rudolph, Hannover/DE, J. Lauth, Tübingen/DE</p>
P01_02	<p>Hybrid Au/MOx Nanostructures for Photoactivated Gas Sensing <u>G. Carelli, Dresden/DE</u>, A. Fery, Dresden/DE, H. Schlicke, Dresden/DE</p>
P01_03	<p>Chromatographic Gas Sensor Stacks: Spatiotemporal VOC Detection for Improved Selectivity <u>L. Mielke, Dresden/DE</u>, A. Fery, Dresden/DE, H. Schlicke, Dresden/DE</p>
P01_04	<p>Electrochemical Multi-Material Additive Manufacturing with Sub-Microscale Resolution <u>S. Sprengel, Oldenburg/DE</u>, T. Zambelli, Zurich/CH, D. Momotenko, Oldenburg/DE, J. Hengsteler, Zurich/CH, P. Zeng, Zurich/CH, A. R. Oliveras, Zurich/CH, M. Z. Zadeh, Oldenburg/DE, W. Wu, Oldenburg/DE, A. Zotov, Zurich/CH, X. Zhu, Brussels/BE, D. Torres, Brussels/BE, J. Ustarroz, Brussels/BE, V. Solovyeva, Oldenburg/DE</p>
P01_05	<p>Exploring hydration effects in photoacid-doped soft materials <u>A. Zieleniewska, Straubing/DE</u></p>
P01_06	<p>Ultrafast Spectroscopic Insights into PCET Driven Excited States of Dinuclear Iridium Complexes <u>N. Maity, Kiel/DE</u>, M. Shee, Kharagpur/IN, F. Temps, Kiel/DE, M. Wächtler, Kiel/DE</p>
P01_07	<p>In-situ small-angle neutron scattering analysis of capillary condensation and evaporation in mesoporous glass <u>C. Gommès, Liege/BE</u>, A. Haidar, Liege/BE, S. Prévost, Grenoble/FR, S. Wellert, Berlin/DE</p>
P01_08	<p>Confinement-Controlled Surface Acidity in Ordered Mesoporous Aluminosilicates <u>S. Itzigebl, Stuttgart/DE</u>, T. Ott, Stuttgart/DE, T. Krol, Stuttgart/DE, M. Amann, Stuttgart/DE, J. R. Bruckner, Stuttgart/DE</p>
P01_09	<p>Synthetic control of gold/semiconductor nanostars <u>L. E. Christoffer, Rostock/DE</u>, T. Peppel, Rostock/DE, K. Boldt, Rostock/DE</p>
P01_10	<p>Anodization of porous anodic aluminum oxide membranes with phosphonic acid <u>C. Twiehaus, Osnabrück/DE</u>, T. Vosmann, Osnabrück/DE, R. B. Wehrspohn, Halle (Saale)/DE, P. Huber, Hamburg/DE, M. Steinhart, Osnabrück/DE</p>
P01_11	<p>Assessing porous stamps for contact lithography <u>N. Schweinitz, Osnabrück/DE</u>, M. Steinhart, Osnabrück/DE</p>
P01_12	<p>Spin-orbit coupling in non-van der Waals 2D materials <u>M. Lokamani, Dresden/DE</u>, G. Bihlmayer, Jülich/DE, G. Michalíček, Jülich/DE, D. Wortmann, Jülich/DE, S. Blügel, Jülich/DE, R. Friedrich, Dresden/DE</p>
P01_13	<p>Structural Evolution of Single-Chain Nanoparticles made from Diblock Copolymers: Insights into Internal Confinement Effects during in silico “Synthesis” <u>F. Plamper, Freiberg/DE</u>, A. Voigt, Freiberg/DE, C. Hübler, Freiberg/DE, S. Schneider, Aachen/DE</p>
P01_16	<p>Interfacial and Grain-Boundary Engineering in ZIF-62 Glass Membranes <u>Z. Zhao, Berlin/DE</u>, A. Mundstock, Hannover/DE, A. Feldhoff, Hannover/DE</p>
P01_17	<p>Ultra-violet to shortwave-infrared transient absorption spectral features of flat PbSe quantum dots in strong confinement <u>J. Unseld, Tübingen/DE</u>, L. Biesterfeld, Tübingen/DE, J. Lauth, Tübingen/DE</p>

P01_18	Designing 2D non-van der Waals Heterostructures <u>A. Nihei, Dresden/DE</u> , T. Barnowsky, Dresden/DE, R. Friedrich, Dresden/DE
P01_19	Tailoring the Surface and Interface of I-III-VI₂ Nanocrystals through Shell Deposition <u>S. Chaudhary, Rostock/DE</u> , K. Boldt, Rostock/DE
P01_20	Surface Functionalization of Non-van der Waals 2D Materials <u>T. Barnowsky, Dresden/DE</u> , M. Christie, Dresden/DE, R. Friedrich, Dresden/DE
P01_21	Confined Water in the Bacterial Translocon SecYEG <u>F. Müh, Linz/AT</u> , L. Nübl, Linz/AT, F. Raubitschek, Linz/AT, E. Sobakinskaya, Linz/AT
P01_22	Utilizing anodic porous alumina membranes as hosts for pharmaceutical ingredients <u>B. Cincin, Osnabrück/DE</u>
P01_23	Ionic conductivity of nanoconfined ionic liquid in metal-organic framework film <u>S. Singh Rana, Berlin/DE</u> , A. Kanj, Karlsruhe/DE, Z. Zhang, Karlsruhe/DE, L. Heinke, Berlin/DE
P01_24	Carrier Diffusion vs. Waveguiding effects in different layered quasi-two-dimensional MAPbI-Perovskites <u>R. Piehler, Rostock/DE</u> , E. Klein, Rostock/DE, R. Lesyuk, Rostock/DE, C. Klinke, Rostock/DE
P01_25	Water Adsorption at Pairs of Brønsted Acid Sites in Zeolites <u>H. Windeck, Berlin/DE</u> , D. Willimetz, Prague/CZ, A. Erlebach, Prague/CZ, C. Heard, Prague/CZ, L. Grajciar, Prague/CZ, F. Berger, Berlin/DE, J. Sauer, Berlin/DE
P01_26	A ring-confined dimetallic dyad mimicking Photosystem I <u>K. P. Zois, Vienna/AT</u> , B. Dietzek-Ivanšić, Jena/DE, S. Rau, Ulm/DE, L. González, Vienna/AT, M. Müßler, Ulm/DE, L. Blechschmidt, Jena/DE, L. Zedler, Jena/DE, K. Mengele, Ulm/DE
P01_27	Highly Yb³⁺-doped core/shell upconversion nanocrystals <u>L. Birk, Osnabrück/DE</u> , M. Haase, Osnabrück/DE
P01_28	Intra- and Post-Synthesis Optimization of α-NiS Nanoparticles <u>O. Krüger, Hamburg/DE</u> , N. Bigall, Hamburg/DE, D. Dorfs, Hamburg/DE
P01_29	Quaternary copper sulfide-based nanocrystals and their gel-like structures <u>P. J. Thomsen, Hamburg/DE</u> , N.-C. Bigall, Hamburg/DE
P01_30	Absorption and Response Properties of Molecules Coupled to Optical Quantum Cavities with Coupled Cluster Theory <u>S. Góger, Saarbrücken/DE</u> , L. Monzel, Saarbrücken/DE
P01_31	Formation of Three-Dimensional Cross-Linked Polymer Networks Studied by Single Molecule Tracking <u>J. Owens, Aachen/DE</u> , D. Malsbenden, Aachen/DE, J. Lerch, Aachen/DE, L. Burow, Aachen/DE, S. Herres-Pawlis, Aachen/DE, D. Wöll, Aachen/DE
P01_32	Steric Confinement for Reactivity and Selectivity in Organolithium and Heterocyclic Chemistry <u>A. Antonov, Regensburg/DE</u>

TOPIC 02: 2D-Materials

P02_01	<p>Synthesis of magnetic 2D heterostructured nanoparticles <u>L. Schoske, Hamburg/DE</u>, H. Borg, Hannover/DE, I. Morales, Hannover/DE, C. Wesemann, Tokyo/JP, R. T. Graf, Hannover/DE, D. Dorfs, Hamburg/DE, N. C. Bigall, Hamburg/DE</p>
P02_02	<p>A flow reactor synthesis of CdSe semiconductor nanoplatelets <u>T. Stoebeke, Hamburg/DE</u>, L. Schoske, Hamburg/DE, J. I. M. Funk, Hamburg/DE, N.-C. Bigall, Hamburg/DE</p>
P02_03	<p>MoS₂ and WS₂ nanowalls with tailored wetting properties <u>R. Ennaciri, Jena/DE</u>, C. Neumann, Jena/DE, A. Turchanin, Jena/DE, M. Zerdani, Jena/DE, M. T. Figge, Jena/DE, C. M. Svensson, Jena/DE</p>
P02_04	<p>Photoelectrochemical Functionalisation of Graphene <u>L. Feuerstein, Dresden/DE</u>, T. Nagel, Fürth/DE, K. Gerein, Fürth/DE, F. Hauke, Fürth/DE, I. M. Weidinger, Dresden/DE</p>
P02_05	<p>Modelling Confined High-Entropy Materials <u>C. C. Er, Dresden/DE</u>, R. Friedrich, Dresden/DE</p>
P02_06	<p>On-Surface Synthesis of 2D Conjugated Organic Polymers on Oxide Single Crystal Surfaces <u>A. R. von Seggern, Oldenburg/DE</u>, C. Groothuis, Oldenburg/DE, L. Mohrhusen, Oldenburg/DE</p>
P02_07	<p>Preparation and Characterization of Photoswitchable Carbon Nanomembranes <u>V. Müller, Jena/DE</u>, D. Hüger, Jena/DE, C. Neumann, Jena/DE, A. Turchanin, Jena/DE</p>
P02_08	<p>Solution-Based Synthesis and Characterization of 1D and 2D Tin Telluride Nanostructures <u>M. Rittner, Hamburg/DE</u>, A. Mews, Hamburg/DE</p>
P02_09	<p>Stimulated Emission from 2D CdSe/CdS Nanoplatelets Integrated in a Liquid-Core Fiber <u>D. A. Rudolph, Hannover/DE</u>, V. Adolfs, Hannover/DE, A. Antanovich, Hannover/DE, S. Spelthann, Hannover/DE, D. H. Chau, Hannover/DE, M. Chemnitz, Jena/DE, M. Schmidt, Jena/DE, M. Steinke, Hannover/DE, J. Lauth, Tübingen/DE</p>
P02_10	<p>Intra- and Interlayer Excitonic Finestructure of the Two-Dimensional Perovskite PEA₂PbI₄ <u>P. Grenzer, Würzburg/DE</u>, F. Lie, Enschede/NL, K. Eckstein, Würzburg/DE, T. Hertel, Würzburg/DE, L. Leppert, Enschede/NL</p>
P02_11	<p>First-Principles Investigations of Charge Transfer and Bandgap Engineering in Functionalised 2H-MoS₂ <u>S. Ray, Berlin/DE</u>, B. Paulus, Berlin/DE</p>

TOPIC 03: Biophysical Chemistry and Biophotonics

P03_01	Unified Solvothermal Synthesis of Size-Uniform Alkali Niobate and Tantalate Nanocrystals for Comparative SHG/THG Studies <u>V. Rosner, Osnabrück/DE</u> , J. Klein, Nordhausen/DE, K. Kömpe, Osnabrück/DE
P03_02	Membrane organoid chips for programmable growth of stem cells <u>E. Schäfer, Osnabrück/DE</u> , C. You, Osnabrück/DE, L. Tveriakhina, Osnabrück/DE, M. Steinhart, Osnabrück/DE
P03_03	Condensates, Aggregates or Both? Thz Calorimetry Puts the Spotlight on Water and Reveals the Nature of Biomolecular Condensates <u>R. V. Teope, Bochum/DE</u> , M. G. Herrera, Bochum/DE, S. Naqvi, Bochum/DE, J. Tatzelt, Bochum/DE, K. Winklhofer, Bochum/DE, M. Havenith, Bochum/DE
P03_04	Salt Mediated Softening of Confined Water in Biomolecular Condensates <u>E. M. Adams, Dresden/DE</u> , A. Czajkowski, Dresden/DE
P03_05	Optical Detection of Inflammation Markers with Chemically Tailored Bionanosensors <u>C. Derichsweiler, Duisburg/Bochum/DE</u> , J. Stegemann, Duisburg/Bochum/DE, J. Ackermann, Duisburg/DE, S. Herbertz, Duisburg/DE, S. Kruss, Duisburg/Bochum/DE
P03_06	Thermodiffusion as a Probe of Hydrophilicity in Alkyl-Substituted Ammonium Salts <u>B. A. Rudani, Jülich/DE</u> , H. Kriegs, Jülich/DE, S. Wiegand, Jülich/DE

TOPIC 04: Catalysis

P04_01	Photoflow Reactors for Polyampholytic Hydrogels: Towards Scalable Noble Metal-Free Light-Driven Hydrogen Evolution <u>D. Ghosh, Jena/DE</u> , F. Schacher, Jena/DE
P04_02	In-situ Raman Studies on 2D Cobalt Porphyrin-based Covalent Organic Frameworks for Electrochemical CO₂ Reduction <u>A. Joseph, Dresden/DE</u> , I. M. Weidinger, Dresden/DE, A. De, Dresden/DE
P04_03	Implemented High-Purity Reactor for Nanostar Photocatalysis <u>L. Möllmann, Rostock/DE</u> , T. Peppel, Rostock/DE, K. Boldt, Rostock/DE
P04_04	Partial selective oxidation of 2-propanol on Co₃O₄(111) and VOx/Co₃O₄(111) model catalysts: solvent and dopant effects <u>P. Kohlmorgen, Kiel/DE</u> , P. Hubert, Kiel/DE, J. Smyczek, Kiel/DE, C. Schröder, Kiel/DE, M. Galinski, Kiel/DE, S. Schaueremann, Kiel/DE
P04_05	Single Atom Alloy Catalysis for Selective Non-Oxidative Butanol Dehydrogenation: From Pd/Cu(111) Single Crystals to Pd/Cu Nanoparticles Supported on Al₂O₃ <u>P. Fröhlich, Kiel/DE</u> , P. Hagg, Kiel/DE, J. Smyczek, Kiel/DE, C. Schröder, Kiel/DE, S. Appelfeller, Lund/SE, K. Neyman, Barcelona/ES, S. Schaueremann, Kiel/DE
P04_06	Study of Atomically Precise Nanocluster/Oxide Interface for Efficient Electrocatalysis <u>M. K. Sikdar, Rostock/DE</u> , T. R. Gazi, Kharagpur /IN, P. Sardar, Kharagpur /IN, A. Roy, Kharagpur /IN, I. Chakraborty, Kharagpur /IN
P04_07	Plasmon-driven Suzuki–Miyaura cross-coupling reactions: role of the generated non-thermal charge carriers <u>R. M. Radwan, Potsdam/DE</u> , I. Bald, Potsdam/DE
P04_08	Unveiling Key Descriptors for CO Oxidation on Nanoporous Gold <u>S. Schiewelbein, Bremen/DE</u> , M. Bäumer, Bremen/DE, R. Moreira, Bremen/DE

P04_09	Unexpected selectivity in alcohol cross-coupling on Au(332) J. M. Correa Hoyos, Berlin/DE, B. Switon, Berlin/DE, A. Butzmann, Berlin/DE, W. Riedel, Berlin/DE, T. Risse, Berlin/DE
P04_10	Influence of Ligands on the Photocatalytic Reduction of 4 Nitrophenol by Gold Nanoparticles J. Manglani-Dreßler, Berlin/DE, C. Pacholski, 13353/DE
P04_11	Investigation of nitric oxide reduction over ceria (CeO₂) catalysts using UHV-IRRAS and DRIFTS techniques A. Essa, Eggenstein-Leopoldshafen/DE, L. Bolz, Eggenstein-Leopoldshafen/DE, Z. Yu, Eggenstein-Leopoldshafen/DE, A. Nefedov, Eggenstein-Leopoldshafen/DE, Y. Wang, Eggenstein-Leopoldshafen/DE, C. Wöll, Eggenstein-Leopoldshafen/DE

TOPIC 05: Electrochemistry

P05_01	Merging electrochemistry with biocatalysis in one-pot processes T. Bookholt, Osnabrück/DE, J. Buddeberg, Bielefeld/DE, H. Gröger, Bielefeld/DE, H. Schäfer, Osnabrück/DE
P05_02	Exchange Current Densities of Catalyst Nanoparticles on Photoelectrodes from Photocurrent Spectroscopy M. Nussör, Tübingen/DE, E. A. Schmitt, Tübingen/DE, M. Diecke, Tübingen/DE, M. M. May, Tübingen/DE
P05_03	(Photo-) Electrochemical Deposition of Silicon from Ionic Liquids M. Diecke, Tübingen/DE, S. Hemmecke, Tübingen/DE, M. Flieg, Tübingen/DE, E. A. Schmitt, Tübingen/DE, M. M. May, Tübingen/DE
P05_05	Electrochemical recycling of epoxy resin-based carbon fibre using methanol as electrolyte P. Ly, Dresden/DE, J. Scheel, Dresden/DE, M. M. Devasis, Dresden/DE, M. Liebscher, Dresden/DE, I. M. Weidinger, Dresden/DE
P05_06	Meeting at the Interface : Promoting Carbonate Reduction via Ion-Surfactant Synergy S. Bharali, Bochum/DE, W. Chen, Bochum/DE, N. S. Wichmann, Bochum/DE, X. Yu, Bochum/DE, S. Pezzotti, Paris/FR, M. Havenith, Bochum/DE
P05_07	Frugal Catalysts by Design. 3D Printing Carbonized Biomass into Functional Electrodes T. Gottwald, Bremen/DE, N. Dami, Bremen/DE, T. M. Gesing, Bremen/DE, M. Bäumer, Bremen/DE, R. Moreira, Bremen/DE
P05_08	Electrochemical investigation of the protective role of redox chains (Tyr/Trp) in complete oxygen reduction: a case of small laccase (SLAC) C. Scharbach, Bonn/DE, H. Pitz, Bonn/DE, P. Kielb, Bonn/DE
P05_09	Electrochemical Insights into the Radical Scavenging Mechanism of DOPA Residues in Collagen Fibers A. F. Ahmed, Bonn/DE, F. Gräter, Mainz/DE, P. Kielb, Bonn/DE
P05_10	Early-Stage Nucleation in Electrochemical Atomic Layer Deposition: Se Deposition on Au(111) S. Reindl, Erlangen/DE, M. S. Ayub, Erlangen/DE, R. Hübsch, Erlangen/DE, Y. Lykhach, Erlangen/DE, O. Brummel, Erlangen/DE, T. Retzer, Erlangen/DE, J. Libuda, Erlangen/DE
P05_11	Impact of Channel Length of Conductive Metal-Organic Framework Films on Charge Transport in Nanoporous Electric Double-Layer Capacitors P. Meier, Berlin/DE, A. Bhatt, Berlin/DE, Y. Liu, Karlsruhe/DE, L. Heinke, Berlin/DE
P05_12	Morphology-Dependent Assembly of PbS Quantum Dots into Hydrogel Network S. Saha, Hamburg/DE, D. Dorfs, Hamburg/DE, N. Bigall, Hamburg/DE

P05_13	Semiconductor Nanoparticle-based Gels as Photoactivated Gas Sensors <u>J.-N. Beyer, Hamburg/DE</u> , T. Vossmeier, Hamburg/DE, N.-C. Bigall, Hamburg/DE
P05_14	Tuning the Energy Release in Molecular Solar Thermals via Substituent Position and Autocatalytic Switching <u>Z. Hussain, Erlangen/DE</u> , E. Franz, Erlangen/DE, A. Müller, Heidelberg/DE, N. Oberhof, Heidelberg/DE, K. Moth-Poulsen, Barcelona/ES, H. Hölzel, Gießen/DE, O. Brummel, Erlangen/DE, J. Libuda, Erlangen/DE
P05_15	(Spectro-) Electrochemistry of Colloidal MoSe₂ Nanosheets <u>S. Westendorf, Tübingen/DE</u> , O. Strolka, Tübingen/DE, J. Lauth, Tübingen/DE, M. Scheele, Tübingen/DE

TOPIC 06: Energy Storage Materials

P06_01	Unraveling the correlation between populated site energies, activation barriers and saddle point energies in solid ion conductors <u>M. Schäfer, Marburg/DE</u> , M. A. Badragheh, Darmstadt/DE, M. Vogel, Darmstadt/DE, K.-M. Weitzel, Marburg/DE
P06_02	In-Situ Activation of a Monolithic SrTiO₃ Single Crystal for Room Temperature Hydrogen Sensing <u>T. Kassubek, Marburg/DE</u> , K. Rein, Marburg/DE, K.-M. Weitzel, Marburg/DE
P06_03	The influence of the Ga-ions on the charge separation processes for in operando quantum dots-based solar cells. <u>D. Sychev, Dresden/DE</u> , A. Senina, Dresden/DE, F. Roeder, Dresden/DE, A. Lubk, Dresden/DE, F. Paulus, Dresden/DE, I. Hermes, Dresden/DE

TOPIC 07: Reaction Kinetics and Dynamics

P07_01	Low-energy Electron Attachment to Nimorazole and 2-bromo-5-nitro-thiazole: Effects of Microhydration <u>G. Schöpfer, Innsbruck/AT</u> , V. T. T. Nguyen, Innsbruck/AT, T. Lob, Innsbruck/AT, S. Denifl, Innsbruck/AT, M. Ončák, Innsbruck/AT
P07_02	ReaxMD: Tracking Atoms in Reactive Molecular Dynamics <u>L. Álvarez, Hannover/DE</u> , R. Buechel, Hannover/DE, K. Vogiatzis, Knoxville/US, I. Frank, Hannover/DE
P07_03	Ab-Initio Simulation of Photoreactions <u>R. Büchel, Hannover/DE</u> , L. Alvarez Figueroa, Hannover/DE, I. Frank, Hannover/DE
P07_04	Molecular Clustering and Their Release Under Nanoconfinement in the Pores of metal Organic Framework <u>A. Pushpa Balakrishnan, Berlin/DE</u> , L. Heinke, Berlin/DE
P07_05	Understanding the Mechanism of Thermally Activated Delayed Fluorescence in Emitters of Donor-Acceptor Type <u>K. M. Knötig, Siegen/DE</u> , T. Lenzer, Siegen/DE, K. Oum, Siegen/DE
P07_06	The Effect of Doping on the Reduction-induced Structural Change of LaMnO_{3+δ} <u>L. Joseph, Koblenz/DE</u> , S. Mascotto, Koblenz/DE, M. D'Arienzo, Milan/IT, S. Mostoni, Milan/IT
P07_07	Investigating protection mechanisms of Lytic polysaccharide monoxygenases against oxidative inactivation - The role of Tyr/Trp chains <u>F. H. Pilz, Bonn/DE</u> , P. Kielb, Bonn/DE
P07_08	Photophysical investigations of an organic dye for perovskite solar cell applications with optical spectroscopy <u>S. M. Stepping, Uppsala/SE</u> , L. Hammarström, Uppsala/SE, G. Boschloo, Uppsala/SE

P07_09	Intrinsic and Solvent-Driven Effects on Energy Barriers in Krohnke, Schiff Base, and Knoevenagel Reactions. <u>L. Lagan, Görlitz/DE</u>
P07_10	Single Molecule Force Spectroscopy (SMFS) of Organometallic Rhodium-π Complexes <u>M. Rainer, Innsbruck/AT, S. F. Wörz, Innsbruck/AT, H. Zhang, Haifa/IL, C. E. Diesendruck, Haifa/IL, M. K. Beyer, Innsbruck/AT</u>
P07_11	Experimental Indication of Regimes of Heterogeneous and Homogeneous Nucleation of Carbon Dioxide Gas-Hydrates <u>B. Rathke, Bremen/DE, L. Pereira, Bremen/DE</u>

TOPIC 08: Spectroscopy

P08_01	Substrate-Assisted Cathodoluminescence <u>S. Ebel, Odense/DK, A. Mortensen, Odense/DK, S. Morozov, Odense/DK</u>
P08_02	High-resolution frequency comb spectroscopy of the ν_8 CH₂-wagging band of dibromomethane isotopologues <u>I. Sadiq, Bochum/DE, A. Balashov, Umeå/SE, A. Hjältén, Umeå/SE, O. Egorov, Tomsk/RU, M. Rey, Reims/FR, A. Foltynowicz, Umeå/SE</u>
P08_03	Photodissociation Spectroscopy and Photochemical Hydrogen Evolution in Al⁺(H₂O) <u>M. K. Beyer, Innsbruck/AT, D. Jank, Innsbruck/AT, M. Reimann, Innsbruck/AT, M. Ončák, Innsbruck/AT, C. van der Linde, Innsbruck/AT</u>
P08_04	Charge-carrier separation in colloidal nanostructures under illumination measured by Kelvin probe force microscopy <u>S. Rolfs, Hamburg/DE, N. Giese, Hamburg/DE, J. Ahrens, Hamburg/DE, T. Kipp, Hamburg/DE, A. Mews, Hamburg/DE</u>
P08_05	Electronic States of Coordinatively Saturated Transition Metal Complexes in the Gas Phase <u>M. Reimann, Innsbruck/AT, M. Ončák, Innsbruck/AT, M. K. Beyer, Innsbruck/AT</u>
P08_06	How fluorination alters local thermodynamic properties of aqueous alcohol solutions <u>S. Schulke, Bochum/DE, E. Casalini, Duisburg/DE, J. Kaur, Bochum/DE, S. Skoko, Duisburg/DE, G. Schwaab, Bochum/DE, A. Vila Verde, Duisburg/DE, M. Havenith, Bochum/DE</u>
P08_07	Understanding Vibrational Strong Coupling through non-linear IR spectroscopy <u>H. Poulou, Potsdam-Golm/DE, Y. Pfeifer, Potsdam-Golm/DE, T. Stensitzki, Potsdam-Golm/DE, M. Noell, Potsdam-Golm/DE, A. Majlesi, Potsdam-Golm/DE, W. Koopman, Potsdam-Golm/DE, C. Henkel, Potsdam-Golm/DE, H. M. Müller-Werkmeister, Potsdam-Golm/DE</u>
P08_08	Using Time-Resolved FTIR-Spectroscopy for Tracing Photoinduced Dynamics and Identifying Involves Intermediates <u>C. Rehhagen, Rostock/DE, L. Kruse, Rostock/DE, R. Ludwig, Rostock/DE</u>
P08_09	Rare encounters with benzonitrile: benchmarking structures, binding energies, and electric field gradients in noble-gas van der Waals complexes <u>J. Fasse, Göttingen/DE, B. Hartwig, Göttingen/DE, W. Mäde, Göttingen/DE, D. Obenchain, Göttingen/DE</u>
P08_10	Halogen Bonds in Rotational Spectroscopy: Mesomeric and Inductive Effects <u>J. N. Hasselhorn, Göttingen/DE, B. Hartwig, Göttingen/DE, D. A. Obenchain, Göttingen/DE</u>
P08_11	Quantification of Halogen Bond Donor Strength by Rotational Spectroscopy <u>J. Hasselhorn, Göttingen/DE, B. Hartwig, Göttingen/DE, D. A. Obenchain, Göttingen/DE</u>
P08_12	Investigations of H-Bonding in Dicarboxylic acid based Ionic liquids <u>M. Azhar, Rostock/DE, R. Ludwig, Rostock/DE</u>

P08_13	<p>CuS Nanoparticle Grating for Directional NIR Quantum Dots Photoluminescence Enhancement <u>V. Alabusheva, Dresden/DE</u>, V. Zakomirnyi, Troyes/FR, S. Seçkin, Dresden/DE, G. Carelli, Dresden/DE, V. Shilovskikh, Dresden/DE, V. Lesnyak, Dresden/DE</p>
P08_14	<p>Characterization of Chain Transfer Agents for RAFT Polymerization on the Gold Nanoparticle Surface <u>N. Deepak, Potsdam/DE</u>, A. H. Esfahani, Potsdam/DE, S. Kogikoski Jr., Potsdam/DE, M. Hartlieb, Potsdam/DE, I. Bald, Potsdam/DE</p>
P08_15	<p>Temperature dependent spectroscopy of Ag₂S nanoparticles for bioimaging <u>L. Schindelhauer, Hamburg/DE</u>, C. Strelow, Hamburg/DE, T. Kipp, Hamburg/DE, A. Mews, Hamburg/DE, B. Juárez, Madrid/ES</p>
P08_16	<p>(Multi)-Exciton Dynamics in Mixed CdSe Quantum Dot Thin Films <u>A. Prax, Kiel/DE</u>, R. Baruah, Kiel/DE, M. Wächtler, Kiel/DE</p>
P08_17	<p>Solvation shell Spectroscopy of Supported Lipid Bilayers <u>B. Moussa, Bochum/DE</u>, B. Justesen, Bochum/DE, T. Günther-Pomorski, Bochum/DE, P. B. Petersen, Bochum/DE</p>
P08_18	<p>First Measurements and Calibration for Measuring the Electrochemical Impedance Spectroscopy of Liquid Substances <u>C. Grau Turuelo, Dresden/DE</u>, A. S. Hashim, Dresden/DE, C. Breitkopf, Dresden/DE</p>
P08_19	<p>Light-induced proton transfer and its impact on membrane dynamics in amphiphile-modified GUVs <u>S. S. Mohanty, Jena/DE</u>, S. R. Bongu, jena/DE, A. Chettri, Potsdam/DE, A. Banerjee, Jena/DE, S. Buzhala, Jena/DE, B. Dietzek-Ivanšić, Jena/DE</p>
P08_20	<p>Photoactive Neutral Three-Coordinate Cu(I) Complexes of Anionic N-Heterocyclic Carbenes <u>T. F. Borowski, Braunschweig/DE</u>, L. E. Burmeister, Braunschweig/DE, L. J. Groth, Braunschweig/DE, P. R. Meinhold, Braunschweig/DE, J. P. Zurwellen, Braunschweig/DE, D. Bockfeld, Braunschweig/DE, R. Frank, Braunschweig/DE, M. Karnahl, Braunschweig/DE, M. Tamm, Braunschweig/DE, S. Tschierlei, Braunschweig/DE</p>
P08_21	<p>Tuning of Arsenic Corrole Complexes by Axial Coordination: From Photophysics to Photosensitization <u>M. Brandstätter, Braunschweig/DE</u>, H. Peters, Braunschweig/DE, A. Riabchunova, Braunschweig/DE, M. Karnahl, Braunschweig/DE, M. Bröring, Braunschweig/DE, S. Tschierlei, Braunschweig/DE</p>
P08_22	<p>Bright, Photostable Alumina-coated Perovskite nanocrystals <u>M. T. Duong, Hamburg/DE</u>, P. Reiss, Grenoble/FR, G. Nogues, Grenoble/FR, N. C. Bigall, Hamburg/DE</p>
P08_23	<p>Unexpected Sign Inversion of the CD and CPL Response of Chiral Copolymer Thin Films by Tuning the Thickness and Annealing Conditions <u>V. Schumacher, Siegen/DE</u>, D. Gust, Siegen/DE, M. Morgenroth, Siegen/DE, M. Scholz, Siegen/DE, K. Oum, Siegen/DE, T. Lenzer, Siegen/DE, J.-C. Mulatier, Lyon/FR, D. Pitrat, Lyon/FR, L. Guy, Lyon/FR</p>
P08_24	<p>Probing CO₂ Adsorption and Transport in Zeolites Using Electrochemical Impedance Spectroscopy <u>A. S. Hashim, Dresden/DE</u>, C. Grau Turuelo, Dresden/DE, C. Breitkopf, Dresden/DE</p>
P08_25	<p>Unraveling Quantum Effects of Flexible Molecules in Superfluid Solvents <u>K. Leitmann, Bochum/DE</u>, H. Forbert, Bochum/DE, D. Marx, Bochum/DE</p>
P08_26	<p>Analyzing Microsolvation Shell Buildup of Helium Around the Zundel Cation Using Highly Accurate Path Integrals Simulations Based on Machine Learning Potentials <u>E. Gil Olaria, Bochum/DE</u>, C. Schran, Cambridge/GB, H. Forbert, Bochum/DE, D. Marx, Bochum/DE</p>
P08_27	<p>Electrochemical Increase of Carbon Nanotube Fluorescence <u>J. A. C. Wartmann, Bochum/DE</u>, S. Kruss, Bochum/DE</p>

P08_28	Impact of Surface Acidity, Hydration, and Temperature on Organic Guest–Host Interactions in Mesoporous Silica I. G. Shenderovich, Regensburg/DE,
P08_29	Insight into Excited State Dynamics of Photooxidised PM6:Y6 Bulk-Heterojunction: Deposited via Langmuir Schaefer Deposition Technique <u>J. Bisht, Jena/DE</u> , Y. T. Gerasea, Jena/DE, M. Presselt, Jena/DE, B. Dietzek-Ivanšić, Leipzig/DE
P08_30	Light-Triggered Proton Transfer in Biomimetic Membranes <u>A. Banerjee, Jena/DE</u> , S. S. Mohanty, Jena/DE, S. R. Bongu, Jena/DE, B. Dietzek-Ivanšić, Leipzig/DE
P08_31	Photoactive nanofibres as materials for light driven catalysis. <u>M. S. Puthanagady, Jena/DE</u> , N. Vashistha, Jena/DE, J. H. Tran, Ulm/DE, B. Dietzek-Ivanšić, Jena/DE, M. Anjass, Jena/DE
P08_32	"Ultrafast photodynamics of photoresponsive amphiphiles in giant unilamellar vesicles" <u>S. Buzhala, Jena/DE</u> , S. S. Mohanty, Jena/DE, A. Banerjee, Jena/DE, S. R. Bongu, Jena/DE, B. Dietzek-Ivanšić, Jena/DE
P08_33	Probing Electrode–Electrolyte Interfaces in Prussian Blue Analogues for Sodium-Ion Batteries Using Vibrational Sum Frequency Generation (VSFG) Spectroscopy <u>A. Sharma, Jena/DE</u> , S. Reddy Bongu, Jena/DE, R. De, Columbus/US, B. Dietzek-Ivanšić, Jena/DE
P08_34	Tuning of excited state properties of backbone-substituted heteroleptic Copper(II) complexes investigated by time-resolved FTIR spectroscopy <u>K. Rediger, Kaiserslautern/DE</u> , K. J. Haseloff, Braunschweig/DE, M. Karnahl, Braunschweig/DE, S. Tschierlei, Braunschweig/DE, M. Wächtler, Kiel/DE
P08_35	Rotational, vibrational, conformational and diastereomeric dimer cooling of aminoalcohols in soft supersonic expansions <u>E. Lwin, Göttingen/DE</u> , M. J. Gözl, Göttingen/DE, N. O. B. Lüttschwager, Göttingen/DE, M. A. Suhm, Göttingen/DE
P08_36	Microhydration of substituted pyrazoles <u>F. Knüppe, Göttingen/DE</u> , E. Lwin, Göttingen/DE, M. A. Suhm, Göttingen/DE
P08_37	OH NO! - Investigating the interactions between TEMPO and large halogenated alcohols <u>E. Sennert, Göttingen/DE</u> , M. A. Suhm, Göttingen/DE
P08_38	Mapping the emissive surface states of graphene quantum dots in the energy landscape with metal cations <u>S. Burai, Kiel/DE</u> , J. Boehmfeld, Kaiserslautern/DE, M. Wächtler, Kiel/DE
P08_39	The influence of surface state bands on the optical properties of 2D Bi₂Se₃ nanoplatelets <u>J. Vliem, Tübingen/DE</u> , S. A. Cayan, Ghent/BE, R. R. Reho, Luxemburg City/LU, A. R. Botello-Méndez, Utrecht/NL, P. Geiregat, Utrecht/NL, Z. Zanolli, Utrecht/NL, D. Vanmaekelbergh, Utrecht/NL, A. Baserga, Milan/IT, R. Kumar, Milan/IT, G. Cerullo, Milan/IT, M. Scheele, Tübingen/DE
P08_40	Surface structure of Cu/CeO₂ nanoparticles probed by CO surface-ligand infrared spectroscopy (SLIR) <u>Z. Li, Eggenstein-Leopoldshafen/DE</u> , L. Caulfield, Eggenstein-Leopoldshafen/DE, L. Bolz, Eggenstein-Leopoldshafen/DE, Z. Yu, Eggenstein-Leopoldshafen/DE, A. Nefedov, Eggenstein-Leopoldshafen/DE, Y. Wang, Eggenstein-Leopoldshafen/DE, C. Wöll, Eggenstein-Leopoldshafen/DE

TOPIC 09: Surfaces and Interfaces

P09_01	<p>Metal-Organic Framework Thin Films Grown on Functionalized Graphene as Solid-State Ion-Gated FETs <u>A. Chandresh, Berlin/DE</u>, C. Wöll, Karlsruhe/DE, L. Heinke, Berlin/DE</p>
P09_02	<p>Laser Pulse-induced Heating of Nanoparticle-based Cryoaerogels <u>C. Tioka, Hamburg/DE</u>, D. Dorfs, Hamburg/DE, N. Bigall, Hamburg/DE</p>
P09_03	<p>TPD Studies of Metal-Substrate Interactions in LOHCs and Polyfluorinated Compounds <u>S. R. Kachel, Marburg/DE</u>, K. Zoltner, Marburg/DE, L. Neuhaus, Marburg/DE, E. Versok, Marburg/DE, J. M. Gottfried, Marburg/DE</p>
P09_04	<p>Area-selective SAM templating on CoO nanoislands/Au(111) <u>N. Sidorenko, Erlangen/DE</u>, J. Hauner, Erlangen/DE, A. Zerreis, Erlangen/DE, J. Libuda, Erlangen/DE</p>
P09_05	<p>Influence of Halide Counterions on Tetrabutylammonium Films and Interfacial Water at Gold Electrodes <u>N. S. Wichmann, Bochum/DE</u>, J. Kaur, Bochum/DE, W. Chen, Paris/FR, S. Pezzotti, Paris/FR, M. Havenith, Bochum/DE</p>
P09_06	<p>Rotational Dynamics of Single Molecules at the Interfaces of Thin Polymer Films <u>D. Malsbenden, Aachen/DE</u>, D. Marx, Göttingen/DE, O. Nevskiy, Göttingen/DE, J. Enderlein, Göttingen/DE, D. Wöll, Aachen/DE</p>
P09_07	<p>Atomically Defined Photoswitchable Hybrid-Nanostructures Based on Functionalized Norbornadienes, Cobalt Oxide Nanoislands, and Au(111) <u>L. Knörr, Erlangen/DE</u>, J. Hauner, Erlangen/DE, A. Zerreis, Erlangen/DE, O. Brummel, Erlangen/DE, J. Libuda, Erlangen/DE</p>
P09_08	<p>Photosensitizer–Silver Nanoparticle Synergy in PEGDA/Gelatin Hybrid Hydrogels for Antibacterial Photodynamic Therapy <u>T. Şener Raman, Leipzig/DE</u>, M. Kühnert, Leipzig/DE, R. Konieczny, Leipzig/DE, N. Lippmann, Leipzig/DE, A. Kaiser, Leipzig/DE, R. Werdehausen, Leipzig/DE, B. Abel, Leipzig/DE, A. Schulze, Leipzig/DE</p>
P09_09	<p>Preparation and Characterization of PtRu/Ru(10-10) Surface Alloys for Model Electrocatalysis <u>D. Schauermann, Erlangen/DE</u>, R. Hübsch, Erlangen/DE, J. Skvara, Prague/CZ, T. Skala, Prague/CZ, N. Tsud, Prague/CZ, J. Myslivecek, Prague/CZ, O. Brummel, Erlangen/DE, Y. Lykhach, Erlangen/DE, J. Libuda, Erlangen/DE</p>
P09_10	<p>Boosting Protein Extraction from <i>Tetraselmis chui</i> with Enzyme-Functionalized Nylon Membranes <u>T. Schreiber, Leipzig/DE</u>, M. Schmidt, Leipzig/DE, A. Prager, Leipzig/DE, A. Poidevin, Saint-Nazaire/FR, E. Couallier, Saint-Nazaire/FR, A. Schulze, Leipzig/DE</p>
P09_11	<p>Ultrathin macroporous substrates for high-resolution microscopy <u>J. Bergjan, Osnabrück/DE</u>, A. C. Basaran, Osnabrück /DE, Ö. D. Asik, Osnabrück/DE, A. Möller, Osnabrück/DE, K. Cosentino, Modena/IT, M. Steinhart, Osnabrück/DE</p>
P09_12	<p>Insights into Single-Atom Catalysis on Boron Nitride Surfaces: A DFT/AIMD Study <u>L. Carroll, Berlin/DE</u></p>
P09_13	<p>Ferroelectric charge separation studies on sintered BaTiO₃ surfaces <u>K. Neuhauser, Salzburg/AT</u>, G. Zickler, Salzburg/AT, T. Berger, Salzburg/AT, O. Diwald, Salzburg/AT</p>
P09_14	<p>Insights into Heterogeneous Ice Nucleation on the Nanoscale <u>F. Schneider, Bielefeld/DE</u>, L. Klausfering, Bielefeld/DE, R. Pires da Silva, Bielefeld/DE, I. A. Ruiz Alvarado, Paderborn/DE, R. Bechstein, Bielefeld/DE, W. G. Schmidt, Paderborn/DE, A. Kühnle, Bielefeld/DE</p>

P09_15	Secondary crosslinking of thermoresponsive microgels for smart microgel-based membranes <u>J. Runge, Bielefeld/DE</u> , S. Uredat, Bielefeld/DE, A. Gujare, Montpellier/FR, J. Oberdisse, Montpellier/FR, T. Hellweg, Bielefeld/DE
P09_16	Direct Observation of Potential-Dependent Surface State Formation at an Electrochemical Interface via the Optical Anisotropy M. Flieg, Tübingen/DE, M. Guidat, Tübingen/DE, M. May, Tübingen/DE
P09_17	Photochemical Action Plots Uncover Wavelength-Controlled Growth of Polymer Brushes <u>K. Rymsha, Dresden/DE</u> , L. Mérai, Dresden/DE, J. Yadav, Dresden/DE, C. Pester, Dresden/DE, A. Fery, Dresden/DE, Q. A. Besford, Dresden/DE
P09_18	Microviscosity-mapping in Polymer Brushes by Fluorescent Molecular Rotors <u>L. Mérai, Dresden/DE</u> , H. Merlitz, Dresden/DE, Q. A. Besford, Dresden/DE

TOPIC 10: Theory and Data Science

P10_01	Uncovering molecular secrets of deep eutectic solvents <u>S. Zahn, Leipzig/DE</u>
P10_02	Active Learning based Dataset Construction for Neural Network Potentials of Water in 2D Nanoconfinement <u>N. Smith, Hamburg/DE</u> , C. Herrmann, Hamburg/DE
P10_03	OrthoBoXY: A Simpler Way to Compute True Self-Diffusion Coefficients and Viscosities from MD Simulations <u>M. Brandt, Rostock/DE</u> , J. Busch, Rostock/DE, D. Paschek, Rostock/DE
P10_04	Coordination Corrected Enthalpies for the Thermodynamics of Ionic Materials <u>B. Thakur, Dresden/DE</u> , R. Friedrich, Dresden/DE
P10_05	The Electronic Ground State Term of the Group 14 Monofluoride Molecules: A Spin-Orbit Coupling Study <u>D. Andrae, Berlin/DE</u> , J. Pantescu-Lucazeau, Lyon/FR
P10_06	From Atomistic Simulations to Indoor Chemistry: Modeling Diffusion Across Interfaces <u>M. von Domaros, Marburg/DE</u> , R. Thomas, Marburg/DE, P. R. Prabhakar, Irvine/US
P10_07	Automating Multireference Calculations for Building a Database of Electronic Transitions in Astrochemical Compounds <u>M. Gatt, Innsbruck/AT</u> , M. Reimann, Innsbruck/AT, G. Schöpfer, Innsbruck/AT, M. Ončák, Innsbruck/AT
P10_08	Light-Triggered Azobenzene-Bithiophene Nanotrap for Fullerenes <u>O. Guskova, Dresden/DE</u> , D. A. Ryndyk, Dresden/DE
P10_09	Parallel Transport Diabatization with Neural Ordinary Differential Equations <u>M. Hütter, Innsbruck/AT</u> , M. Ončák, Innsbruck/AT
P10_10	Chemical Space Exploration with Artificial “Mindless” Molecules <u>J. Schöps, Bonn/DE</u> , T. Gasevic, Bonn/DE, M. Müller, Bonn/DE, S. Lanius, Berlin/DE, J. Hermann, Berlin/DE, S. Grimme, Bonn/DE, A. Hansen, Bonn/DE

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