BUNSEN-TAGUNG 2022

Understanding Dispersion Interactions in Molecular Chemistry

Justus Liebig University Giessen
September 7-9, 2022

LECTURE SCHEDULE & POSTER LIST

Deutsche Bunsen-Gesellschaft für physikalische Chemie

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN

BUNSEN-TAGUNG 2022

Understanding Dispersion Interactions in Molecular Chemistry
Justus Liebig University Giessen, September 7-9, 2022
www.bunsentagung.de

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EXHIBITORS

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Deutsche Bunsen-Gesellschaft & young Physical Chemists

Exhibition starts at
Thursday 10:20 / 12:00 / 15:30 & Friday 10:20 / 12:20

TABLES OF CONTENT

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LECTURE SCHEDULE

Wednesday, September 7, 2022

16:00 **OPENING CEREMONY** **C112**

OPENING LECTURE **C112**

17:15 Efficient and accurate theoretical treatment of dispersion interactions
S. Grimme, Bonn/DE

19:00 **WELCOME RECEPTION**
Mathematikum & Justus Liebig Museum (registration needed)

Thursday, September 8, 2022, 08:30

PLENARY LECTURE **C112**

08:30 **Dispersion in Solution: What is it Worth?**
S. Cockroft, Edinburgh/GB

THURSDAY MORNING Parallel Sessions 1

Thursday, September 8, 2022, 08:30 - 10.20

C112

KEY TOPIC: Dispersion Interactions

09:20 **Liquid due to Dispersion? Some Superheavy Examples.**
J.-M. Mewes, Bonn/DE , O. R. Smits, Auckland/NZ, P. Schwerdtfeger, Auckland/NZ

09:40 **Stepwise fluorination tunes local hydration shell structure and thermodynamics**
A. Vila Verde, Duisburg/DE , J. Robalo, Berlin/DE, D. M. de Oliveira, West Lafayette/US, L. Streacker, West Lafayette/US, P. Imhof, Erlangen/DE, D. Ben-Amotz, West Lafayette/US

10:00 **The influence of hydrogen bonding and dispersion interaction on the properties of ionic liquids**
R. Ludwig, Rostock/DE , D. H. Zaitsau, Rostock/DE, J. Neumann, Rostock/DE, T. Niemann, Rostock/DE, A. Strate, Rostock/DE, D. Paschek, Rostock/DE, S. P. Verevkin, Rostock/DE

C5a

Spectroscopy

10:00 **Dissecting non-covalent interactions in carboxyl-functionalized ionic liquids exhibiting double and single hydrogen bonds between ions of like charge**
L. Hunger, Rostock/DE , L. Al Sheakh, Rostock/DE, D. H. Zaitsau , Rostock/DE, S. P. Verevkin , Rostock/DE, R. Ludwig, Rostock/DE

KEY TOPIC: Dispersion Interactions

C5b

09:20 **Rotational study of molecular H_2 in dispersive complexes with small aromatic systems**
M. Dohmen, Göttingen/DE , M. Schnell, Hamburg/DE, P. Pinacho, Hamburg/DE, D. Obenchain, Göttingen/DE

09:40 **Competition and cooperation of -OH and π-interactions: Complexes of 2-decalone with water, benzene, and phenol.**
P. Pinacho, Hamburg/DE , S. V. M. Caliebe, Hamburg/DE, M. Schnell, Hamburg/DE

10:00 **A balancing act: Dispersion interactions driving small ketone balance systems**
C. Zimmermann, Göttingen/DE , H. C. Gottschalk, Göttingen/DE, T. L. Fischer, Göttingen/DE, A. Dorst, Göttingen/DE, M. A. Suhm, Göttingen /DE

Reaction Kinetics and Dynamics

C1

09:20 **Condensed phase isomerization through tunneling gateways**
A. Choudhury, Göttingen/DE , J. Devine, Göttingen/DE, S. Sinha, Potsdam/DE, J. A. Lau, California/US, A. Kandratsenka, Göttingen/DE, D. Schwarzer, Göttingen/DE, P. Saalfrank, Potsdam/DE, A. M. Wodtke, Göttingen/DE

09:40 **Tracing organoselenium intermediates in photoreactions**
C. Allacher, Regensburg/DE , R. J. Kutta, Regensburg/DE, D. Grenda, Regensburg/DE, E. Harrer, Regensburg/DE, A. K. Dutta, Regensburg/DE, S. Park, Regensburg/DE, A. Breder, Regensburg/DE, P. Nürnberger, Regensburg/DE

10:00 **Studies on Cluster dynamics below the critical temperature of sulfuric acid nucleation**
S. Celik, Göttingen/DE , J. F. Wilsch, Göttingen/DE, D. Becker, Göttingen/DE, T. Olenius, Norrköping/SE, J. Elm, Aarhus/DK, T. Zeuch, Göttingen/DE

Biophysical Chemistry

C2

09:20 **Dipolar Interactions and Protein Hydration in Highly Concentrated Antibody Formulations**
P. Garidel, Biberach/DE , J. Hartl, Halle/DE

09:40 **Covalent functionalization strategies for near infrared fluorescent carbon nanotube biosensors**
J. T. Metternich, Duisburg/DE , P. Galonska, Bochum/DE, A. Schrage, Bochum/DE, S. Herbertz, Duisburg/DE, S. Kruss, Bochum/DE

10:00 **Exfoliation of near infrared fluorescent silicate nanosheets**
B. Hill, Bochum/DE , G. Selvaggio, Bochum/DE, S. Kruss, Bochum/DE

Thursday, September 8, 2022, 10:20 - 10:40

10:20 **COFFEE BREAK**

EXHIBITION OPEN

THURSDAY MORNING Parallel Sessions 2

Thursday, September 8, 2022, 10:40 - 12:00

KEY TOPIC: Dispersion Interactions **C112**

10:40 **Keynote Lecture: Quantifying London Dispersion using Azobenzene Switches in Solution – Fact or Fake News?**
H. A. Wegner, Giessen/DE

11:20 **Non-Covalent Interactions in Molecular Receptors and Crystals**
M. Stein, Magdeburg/DE , E. Boz, Magdeburg/DE, M. Heimsaat, Magdeburg/DE

11:40 **Investigating the Structure of Azaphenanthrene Dimers by IR/UV Double Resonance Spectroscopy**
T. Preitschopf, Würzburg/DE , X. Miao, Würzburg/DE, F. Sturm, Würzburg/DE, A. K. Lemmens, Nijmegen/NL, R. Mitric, Würzburg/DE, I. Fischer, Würzburg/DE

Spectroscopy **C5a**

10:40 **Online Monitoring of Enantiomeric Ratios by Chirality Recognition in the Gas Phase**
S. Schmahl, Leipzig/DE , H. Westphal, Leipzig/DE, F. Horn, Leipzig/DE, J. Jin, Leipzig/DE, D. Belder, Leipzig/DE, K. R. Asmis, Leipzig/DE

11:00 **A Little Friendly Competition: The Influence of Intramolecular Hydrogen Bonding on the Structure of Metal-Ion-Peptide Complexes and the Impact of Solvation**
K. A. E. Meyer, Madison/US , K. A. Nickson, Madison/US, E. Garand, Madison/US

11:20 **Photoelectron Circular Dichroism in the Photodetachment of Amino Acid Anions**
J. Both, Marburg/DE , P. Krüger, Marburg/DE, K.-M. Weitzel, Marburg/DE

11:40 **New jet-cooled vibrational spectroscopic benchmark data of the cyclic dimer and trimer of formic acid**
A. Nejad, Göttingen/DE , K. Meyer, Madison/US, M. Suhm, Göttingen/DE

KEY TOPIC: Dispersion Interactions — C5b

10:40 **Quantum Effects due to Weak Interactions: A Case Study for Molecular Boron Rotors**
J. Manz, Berlin/DE , T. Grohmann, Berlin/DE, D. Haase, Berlin/DE, D. Jia, Xi'An/CN, S.-D. Li, Taiyuan/CN, X.-Q. Lu, Taiyuan/CN, Y. Yang, Taiyuan/CN

11:00 **Understanding the cooperative interplay of molecular machines embedded in Metal-Organic Frameworks by on-the-fly trained interatomic potentials**
S. Amirjalayer, Münster/DE , E. Kolodzeiski , Münster/DE

11:20 **A time-resolved photoelectron imaging study on the photophysics of the dimers of Benzo(f)quinoline, Benzo(h)quinoline and Phenanthridine**
F. Sturm, Würzburg/DE , C. Stapper, Würzburg/DE, M. Flock, Oberkochen/DE, L. N. Philipp, Würzburg/DE, I. Fischer, Würzburg/DE

11:40 **Marangoni effect-assisted synthesis and investigation of two-dimensional metal aerogels near water-oil interfaces**
P. Khavlyuk, Dresden/DE , A Eychmüller, Dresden/DE, V Shamraienko, Dresden/DE, A Mitrofanov, Dresden/DE

Reaction Kinetics and Dynamics — C1

10:40 **Cryo Kinetics and IR Spectroscopy of N_2 on Tantalum Cluster**
D. V. Fries, Kaiserslautern/DE , A. Straßner, Kaiserslautern/DE, M. P. Klein, Kaiserslautern/DE, M. Huber, Kaiserslautern/DE, M. Luczak, Kaiserslautern/DE, C. Wiehn, Kaiserslautern/DE, M. H. Prosenc, Kaiserslautern/DE, G. Niedner-Schatteburg, Kaiserslautern/DE

11:00 **Interaction of Ruthenium Photosensitizers with Biomolecules Influences the Photophysical Properties of Function Determining Low Lying Triplet States in Photodynamic Therapy.**
A. Chettri, Jena/DE , K. R. A Schneider, Jena/DE, T Yang, Jena/DE, J. A Roque III, Arlington/US, H. D Cole, Arlington/US, C. G Cameron, Arlington/US, S. A. McFarland, Arlington/US, B. Dietzek-Ivanšić, Jena/DE

LECTURE SCHEDULE

THURSDAY MORNING Parallel Sessions 2

Reaction Kinetics and Dynamics — C1

11:20 **Keynote Lecture: Dynamics of the oxygen transfer reaction between carbon dioxide and the tantalum cation Ta^+**
J. Meyer, Kaiserslautern/DE , M. Meta, Kaiserslautern/DE, M. Huber, Kaiserslautern/DE, A. Ayasli, Innsbruck/AT, T. Michaelsen, Innsbruck/AT, R. Wester, Innsbruck/AT

Biophysical Chemistry — C2

11:00 **Controlled amphipathic peptide adsorption by smart, electro-responsive germanium interfaces**
M. Rabe, Düsseldorf/DE , L.-M. Baumgartner, Düsseldorf/DE, A. L. Boyle, Leiden/NL, A. Erbe, Trondheim/NO

11:20 **Time-Resolved Infrared Difference Spectroscopy on Proteins in Living Cells**
L. Goett-Zink, Bielefeld/DE , L. Baum, Bielefeld/DE, T. Kottke, Bielefeld/DE

11:40 **Nitrile IR intensities characterize electric fields and hydrogen bonding in protic, aprotic and protein environments**
J. Kozuch, Berlin/DE , J. Weaver, Stanford/US, J. Kirsh, Stanford/US, S. Boxer, Stanford/US

Theory and Data Science — C103

10:40 **Low scaling Quantum Monte Carlo calculations using subsampling**
J. Feldt, Rostock/DE , A. Bienvenu, Paris/FR, J. Toulouse, Paris/FR, R. Assaraf, Paris/FR

11:00 **Semantic Research Data and Sample Management with CaosDB**
F. Spreckelsen, Göttingen/DE , D. Hornung, Göttingen/DE

11:20 **Energy Transfer and Interaction among Quantum Dot Qubits**
A. Bande, Berlin/DE

11:40 **IDeep Learning for Dimensionality Reduction in Molecular Simulations & Coarse Grained Force Field Development**
Y. Bozkurt Varolgunes, Mainz/DE , J.F. Rudzinski, Mainz/DE

Thursday, September 8, 2022, 12:00 - 12:30

12:00 **LUNCH BREAK**

EXHIBITION OPEN

Thursday, September 8, 2022, 12:30 - 14:30

12:30 **POSTER SESSION PART I – EVEN NUMBERS**
Physics lecture hall building

EXHIBITION OPEN

LECTURE SCHEDULE

Thursday, September 8, 2022, 14:30 - 15:30

KEY TOPIC: Dispersion Interactions — C112

14:30 **Silyl Groups are Strong Dispersion Energy Donors**
L. Rummel, Giessen/DE , P. R. Schreiner, Giessen/DE, H. König, Giessen/DE

14:50 **Tilting the Balance: Stabilising Z-imines via intramolecular Dispersion Interactions and its impact in enantioselective Brønsted acid catalysed transfer hydrogenations**
J. Gramüller, Regensburg/DE , R. M. Gschwind, Regensburg/DE

15:10 **Syntheses and Properties of Diethylphthalane-Incorporated [10]Cycloparaphenylenes**
J. Volkmann, Giessen/DE , H. A. Wegner, Giessen/DE

Spectroscopy — C5a

14:30 **Infrared Photodissociation Spectroscopy of Hydrogen-bonded HFIP Halides Clusters: Conformation and Anharmonicity**
M. Barp, Leipzig/DE , J. Jin, Leipzig/DE, C. Xu, Leipzig/DE, K. Asmis, Leipzig/DE

14:50 **High Resolution Infrared Spectroscopy of Aziridine-2-Carbonitrile**
K. Keppler, Zürich/CH , S. Albert, Zürich/CH, C. Manca Tanner, Zürich/CH, J. Stohner, Wädenswil/CH, M. Quack, Zürich/CH

15:10 **Auger electron spectroscopy of Fulminic acid, HCNO**
M. Gerlach, Würzburg/DE , T. Preitschopf, Würzburg/DE, E. Karaev, Würzburg/DE, H. Lara, Würzburg/DE, D. Mayer, Potsdam/DE, J. Bozek, St. Aubin/FR, R. Fink, Tübingen/DE, I. Fischer, Würzburg/DE

DBG Award Winners — C5b

14:30 **Nernst Haber Bodenstein Award**
Coupling active matter and electrochemistry - galvanophoretic microswimmers
J. Simmchen, Dresden/DE

14:50 **Ewald Wicke Award**
Optimizing Ionic Liquids by Cation Design
D. Rauber, Saarbrücken/DE

15:10 **Honorary Member of the DBG**
Symmetry and Evolution: Molecules in Motion Between Less than Yoctoseconds and More than Days
M. Quack, Zürich/CH

Reaction Kinetics and Dynamics

C1

14:30 **Investigation of the interaction of formic acid with flat and stepped palladium surfaces**
J. Fingerhut, Göttingen/DE , M. Schwarzer, Göttingen/DE, D. Borodin, Göttingen/DE

14:50 **Charge-Transfer Dynamics between Photoexcited CdSe@CdS Nanorods and (Poly)Dopamine**
M. Micheel, Jena/DE , M. Boecker, Mainz/DE, C. Synatschke, Mainz/DE, T. Weil, Mainz/DE, M. Wächtler, Jena/DE

15:10 **Deazaflavin reductive photocatalysis involves excited semiquinone radicals**
R. J. Kutta, Regensburg/DE , A. Graml, Regensburg/DE, T. Neveselý, Prag/CZ, R. Cibulka, Prag/CZ, B. König, Regensburg/DE

Special Symposium "International Year of Glass"

14:30, C2

An ancient material with a rich cultural heritage, glass is more important to modern life than ever before: versatile and easily innovated, it is a potential enabler of the UN 2030 Agenda for Sustainable Development. That is why the UN General Assembly formally declared 2022 as the International Year of Glass (IYOG), celebrating the pivotal role that glass has played in our society for thousands of years. Join these renowned scientists on a journey through the fascinating world of glass:

- PD Dr. Martin Kilo, Fraunhofer Institute for Silicate Research ISC, Bronnbach
- Prof. Dr. Dominique de Ligny, Friedrich Alexander University Erlangen-Nürnberg
- Prof. Dr. Lothar Wondraczek, Friedrich Schiller University Jena

www.iyog2022.org

Theory and Data Science

C103

14:30 **Understanding Organometallic Bonds in On-Surface Ullmann Coupling Reactions by Using the Projected COHP Method**
J. Jung, Giessen/DE , D. Mollenhauer, Giessen/DE

14:50 **Effect of the σ hole orientation on the halogen bonding strength of bromo/iodobenzene on coinage metal(111) surfaces**
P. Henkel, Gießen/DE , K. L. H. Pohl, Gießen/DE, D. Mollenhauer, Gießen/DE

15:10 **Multiscale Simulations for the Computational Spectroscopy of Phytochrome-like Photoreceptors**
C. Wiebeler, Leipzig/DE

LECTURE SCHEDULE

Thursday, September 8, 2022, 15:30 - 15:50

EXHIBITION OPEN

15.30 **COFFEE BREAK**

Thursday, September 8, 2022, 15:50 - 17:30

THURSDAY AFTERNOON Parallel Sessions 2

KEY TOPIC: Dispersion Interactions — C112

15:50 **Unravelling the role of dispersion interactions in molecular crystal structures**
A. A. Auer, Mülheim (Ruhr)/DE , G. Bistoni, Perugia/IT, S. Schulz, Essen/DE, E. Schiavo, Mülheim (Ruhr)/DE, M. Mehring, Chemnitz/DE

16:10 **Tuning hydrogen- and host-guest bonding with small molecular changes – self-assembly at the liquid/solid interface investigated by STM**
R. Reynaerts, Leuven/BE, N. Herrmann, Leuven/BE, K. S. Mali, Leuven/BE, A. Minoia, Mons/BE, D. De Vos, Leuven/BE, S. De Feyter, Leuven/BE

16:30 **Metal–metal interaction of isolated binuclear coinage metal complexes: electronic spectroscopy and photofragmentation**
M. J. P. Schmitt, Kaiserslautern/DE , S. V. Kruppa, Kaiserslautern/DE, R. Israil, Kaiserslautern/DE, W. R. Thiel, Kaiserslautern/DE, R. Diller, Kaiserslautern/DE, W. Klopper, Karlsruhe/DE, C. Riehn, Kaiserlautern/DE

16:50 **Nucleation Enhancement of Butane by Carbon Dioxide, Nitrous Oxide and Propane**
S. Feusi, Zürich/CH , J. Krohn, Zürich/CH, C. Li, Shanghai/CN, R. Signorell, Zürich/CH

17:10 **Multidentate Adsorption of Methylamine on Rutile TiO_2 (110)**
L. Mohrhusen, Oldenburg/DE , L. Gerhards, Oldenburg/DE, D. Hirsch, Oldenburg/DE, T. Klüner, Oldenburg/DE, K. Al-Shamery, Oldenburg/DE

Spectroscopy — C5a

15:50 **Application of Modulation-Excitation Spectroscopy to Unravel the Mechanism of Ethanol Gas Sensing over Au/SnO_2**
M. Pfeiffer, Darmstadt/DE , C. Hess, Darmstadt/DE

16:10 **Water Induced Polymer Reorientation at a Polystyrene/Polyacrylic Acid Surface**
M. E. Encheva, Vienna/AT , X. Li, Mainz/DE, H. J. Butt, Mainz/DE, R. Berger, Mainz/DE, E. H. G Backus, Vienna/AT

16:30 **Ion specific Interactions and Surface Enrichment in Mixed Aerosol**
C. M. Saak, Vienna/AT , S. M. Mika, Vienna/AT, E. H. G. Backus, Vienna/AT

16:50 **Ultrafast Interactions in Dual-Plasmonic Au-CuS Nanocrystals**
A. Niebur, Hannover/DE , P. Bessel, Hannover/DE, D. Kranz, Hannover/DE, D. Dorfs, Hannover/DE, J. Lauth, Tübingen/DE

17:10 **Infrared Action Spectroscopy of Single Nanoparticles in the Gas Phase**
S. Leippe, Leipzig/DE , B. Hoffmann, Leipzig/DE, K. R. Asmis, Leipzig/DE

Agnes Pockels & DFG Session

C5b

15:50 **Investigation of Zeolite Reactivity and Method Development for Accurate Free Energy Calculations**
F. Berger, Berlin/DE

16:10 **Understanding Battery Materials at the Atomic Level Using Neural Network Potentials**
M. Eckhoff, Göttingen/DE

16:30 **All you need is multivariate data – Operando spectroscopy to unravel photocatalytic mechanisms**
C. Müller, Luxembourg/LU

16:50 **Near-infrared spectroscopy of crystalline and amorphous ices**
C. Tonauer, Innsbruck/AT , E.-M. Köck, Innsbruck/AT, R. Henn, Innbruck/AT, C. Huck, Innsbruck/AT, T. Loerting, Innsbruck/AT

17:10 **Funding Opportunities for Early Career Researchers at a Glance**
DFG (Deutsche Forschungsgemeinschaft)

Reaction Kinetics and Dynamics

C1

15:50 **Solvation dynamics and kinetic studies of nascent aqueous iodine atoms and its diffusion-driven products**
Z. Nurekeyev, Hamburg/DE , K. Kubicek, Hamburg/DE, C. Bressler, Hamburg/DE

16:10 **Reversible (photo)chemistry of Cr(0), Mo(0) and W(0) carbonyl complexes**
S. Steiger, Kaiserslautern/DE , P. Boden, Kaiserslautern/DE, P. Di Martino-Fumo, Kaiserslautern/DE, T. Bens, Stuttgart/DE, D. Marhöfer, Kaiserslautern/DE, B. Sarkar, Stuttgart/DE, G. Niedner-Schatteburg, Kaiserslautern/DE

16:30 **Kinetically Driven Shape Control of Colloidal Nanostructures**
K. Boldt, Konstanz/DE , F Enders, Konstanz/DE, D Fischli, Konstanz/DE, M Seybold, Konstanz/DE, S Sutter, Konstanz/DE, J Grings, Konstanz/DE

16:50 **Formation studies and synthesis optimization of Sb_2S_3 nanoparticles**
M. Joschko, Darmstadt/DE , F. Y. Fotue Wafo, Darmstadt/DE, C. Malsi, Darmstadt/DE, J. Rapier, Darmstadt/DE, I. L. Validžić, Belgrade/RS, C. Graf, Darmstadt/DE

17:10 **Femtosecond laser generation of binary metallic oxide nanoparticles for applications in medical imaging diagnosis**
W. Kautek, Vienna/AT , A. Naghilou, Vienna/AT, R. Lahoz, Zaragoza/ES, O. Bomati Miguel, Cádiz/ES, M. Kitzler, Vienna/AT, A. Subotic, Vienna/AT

Transport and Storage

C2

15:50 **Classifying Electrolyte Solutions by Comparing Charge and Mass Transport**
B. Roling, Marburg/DE , J. Kettner, Marburg/DE, V. Miß, Marburg/DE

16:10 **Tailoring charge transport in artificial mixed conducting nanocomposites by surface engineering**
M. T. Elm, Giessen/DE

16:30 **Investigation of charge transport in composite cathodes for solid-state batteries**
P. Minnmann, Giessen/DE , J. Schubert, Giessen/DE, S. Burkhardt, Giessen/DE, F. Richter, Giessen/DE, J. Janek, Giessen/DE

16:50 **Unification of Bulk Storage and Supercapacitive Storage**
C. Xiao, Stuttgart/DE , R. Usiskin, Stuttgart/DE, J. Maier, Stuttgart/DE

17:10 **In-situ Quantification of Chemo-Mechanical Degradation in Solid-State Lithium-Ion Batteries**
R. Ruess, Giessen/DE , G. Conforto, Giessen/DE, D. Schröder, Braunschweig/DE, E. Trevisanello, Giessen/DE, F. H. Richter, Giessen/DE, J. Janek, Giessen/DE

Theory and Data Science

C103

15:50 **Keynote Lecture: Coarse-graining all-atom molecular dynamics into free energies and friction profiles: accessing dynamics on multisecond time scale**
S. Wolf, Freiburg/DE , B. Lickert, Freiburg/DE, M. Jäger, Freiburg/DE, S. Bray, Freiburg/DE, G. Stock, Freiburg/DE

16:30 **Towards an Effective Screening Procedure of Redox-Active Molecules for Organic Polymer Batteries**
A. Achazi, Gießen/DE , D. Mollenhauer, Gießen/DE

LECTURE SCHEDULE

16:50 **From superoxides to singlet-oxygen - A dynamical view on the dissociation mechanism**
D. S. Pietruschka, Gießen/DE , A. Zaichenko, Gießen/DE, M. Richter, Jena/DE, S. Gräfe, Jena/DE, D. Mollenhauer, Gießen/DE

17:10 **The efficient composite DFT method ωB97X-3c and its application as reference for large NCI complexes**
B. Bädorf, Bonn/DE , M. Müller, Bonn/DE, A. Hansen, Bonn/DE, S. Grimme, Bonn/DE

Thursday, September 8, 2022, 18:00 - 20:00

18:00 **POSTER SESSION PART I I – ODD NUMBERS**

Physics lecture hall building

Friday, September 9, 2022, 08:30

PLENARY LECTURE **C112**

08:30 **Probing dispersion interactions using broadband rotational spectroscopy**
M. Schnell, Hamburg/DE

FRIDAY MORNING Parallel Sessions 1

Friday, September 9, 2022, 09:20 - 10:20

KEY TOPIC: Dispersion Interactions **C112**

09:20 **A New Hydrocarbon Balance to Quantify London Dispersion Interactions in Solution**
F. Wilming, Gießen/DE , P. R. Schreiner, Gießen/DE

09:40 **London Dispersion Favors Sterically Hindered Diarylthiourea Conformers in Solution**
M. H. J. Domanski, Giessen/DE , L. Rummel, Giessen/DE, H. Hausmann, Giessen/DE, J. Becker, Giessen/DE, P. R. Schreiner, Giessen/DE

10:00 **Control of the hydrogen bond topology in alcohol-hydroxyester complexes with London dispersion**
M. Lange, Göttingen/DE , E. Sennert, Göttingen/DE, M. A. Suhm, Göttingen/DE

Spectroscopy

C5a

09:20 **Triplet triplet annihilation upconversion by polymeric sensitizers**
K. K. Jha, Jena/DE , A. Prabhakaran, Dublin/IE, T. E. Keyes, Dublin/IE, M. Jäger, Jena/DE, B. Dietzek Ivanšić, Jena/DE

09:40 **Molecular Functionalization of Carbon Nitride Polymers for Light-driven Water Splitting**
C. Li, Jena/DE , I. Krivtsov, Oviedo/ES, C. Adler, Ulm/DE, D. Mitoraj, Ulm/DE, R. Beranek, Ulm/DE, B. Dietzek-Ivanšić, Jena/DE

10:00 **Mechanistic insights into molecular recognition and photophysics of carbon nanotube sensors**
P. Galonska, Bochum/DE , A. Schrage, Bochum/DE, S. S. Nalige, Bochum/DE, L. Sistemich, Bochum/DE, C. Herrmann, Bochum/DE, M. Havenith, Bochum/DE, S. Kruss, Bochum/DE

Reaction Kinetics and Dynamics

C5b

09:20 **Template synthesis of two-dimensional I-III-VI based semiconductor nanocrystals with intensive photoluminescence**
A. Bora, Dresden/DE , A. Prudnikau, Dresden/DE, N. Fu, Dresden/DE, N. Gaponik, Dresden/DE, V. Lesnyak, Dresden/DE

09:40 **Quantum defects as tool to understand exciton dynamics in a fluorescent nanomaterial**
A. Schrage, Bochum/DE , P. Galonska, Bochum/DE, A. Spreinat, Göttingen/DE, M. Dohmen, Göttingen/DE, S. Kruss, Bochum/DE

10:00 **The use of a tertiary solvent mixture to study solvent dynamic effects in the photoinduced electron transfer reaction of excited singlet pyrene and indole**
S. Landgraf, Graz/AT , P. Choto, Chiang Rai/TH, G. Grampp, Graz/AT

Electrochemistry

C1

09:20 **Application of Lithium Metal Anodes in All-Solid-State Batteries - The Role of the Native Passivation Layer**
S.-K. Otto, Giessen/DE , T. Fuchs, Giessen/DE, Y. Moryson, Giessen/DE, J. Janek, Giessen/DE, A. Henss, Giessen/DE

09:40 **Hybrid material approaches for thiophosphate electrolyte-based solid-state batteries**
N. M. Vargas-Barbosa, Münster/DE

09:20 **Failure mechanism and a stack pressure dilemma of the Li metal solid state battery**
J. Duan, Giessen/DE , T. Fuchs, Giessen/DE, A. Henss, Giessen/DE, J. Janek, Giessen/DE

Transport and Storage — C2

09:20 **Keynote Lecture: How well do we understand ion transport in oxides?**
M. Martin, Aachen/DE

10:00 **Li^+ Ion Site Energy Distribution in Lithiumborate**
V. Gunawan, Marburg/DE , Anna Dorfmüller, Marburg/DE, Martin Schäfer, Marburg/DE, K.-M. Weitzel, Marburg/DE

Catalysis — C103

09:20 **Synthesis and Characterization of Hybrid Semiconductor-Metal Nanostructures for Photocatalytical Applications**
M. Dittmar, Hamburg/DE, S. Hentschel, Hamburg/DE, J. Rebmann, Hamburg/DE, T. Kipp, Hamburg/DE, C. Strelow, Hamburg/DE, A. Mews, Hamburg/DE

09:40 **$BiVO_4$ as a colloidal photocatalyst**
M. Wittmann, Dresden/DE , S. Heckel, Dresden/DE, J. Simmchen, Dresden/DE

10:00 **$InPt/In_2O_3$ Aerogels for Methanol Steam Reforming**
L. Thoni, Dresden/DE , N. Köwitsch, Chemnitz/DE, M. Armbrüster, Chemnitz/DE, A. Eychmüller, Dresden/DE

Friday, September 9, 2022, 10:20 - 10:40

10:20 **COFFEE BREAK**

EXHIBITION OPEN

Friday, September 9, 2022, 10:40 - 12:20

KEY TOPIC: Dispersion Interactions — C112

10:40 **Solvation and Aggregation under the Influence of Dispersion Interaction in Superfluid Helium Nanodroplets**
A. Slenczka, Regensburg/DE , J. Fischer, Regensburg/DE, F. Schlaghaufer, Regensburg/DE

11:00 **Two-component benchmarking: dispersive effects in the chlorine nuclear electric quadrupolar coupling tensor observed via rotational spectroscopy of weakly-bound complexes**
D. Obenchain, Göttingen/DE , D. Fedosov, Göttingen/DE, M. Dohmen, Göttingen/DE

11:20 **The role of dispersion interactions for metal-metal and metal-aryl contacts of crystalline Bi and Sb compounds**
G. Jansen, Essen/DE , S. Schulz, Essen/DE, F. van der Vight, Essen/DE, A. Gelhaar, Essen/DE

11:40 **Keynote Lecture: Four Experimental Systems that Test Dispersion Interactions in the Gas Phase and Solution**
P. Chen, Zürich/CH , R. Pollice, Zürich/CH, M. Bot, Zürich/CH, V. Gorbachev, Zürich/CH, A. Tzybisova, Zürich/CH, L. Miloglyadova, Zürich/CH

Spectroscopy — C5b

10:40 **Surface Treatment of Colloidal 2D Lead Chalcogenide NPLs for Emission Enhancement at Telecom Wavelengths**
L. Biesterfeld, Hannover/DE , L. F. Klepzig, Hannover/DE, A. Niebur, Hannover/DE, J. Lauth, Tübingen/DE

11:00 **Colloidal 2D Lead Chalcogenide Nanoplatelets: Efficient Photoluminescence by Post-synthetic Ligand Treatment**
L. F. Klepzig, Hannover/DE , L. Biesterfeld, Hannover/DE, A. Niebur, Hannover/DE, J. Lauth, Hannover/DE

11:20 **Towards understanding photon absorption and emission in MgAl layered double hydroxide**
B. Gevers, Pretoria/ZA , E. Roduner, Stuttgart/DE, F. Labuschagné, Pretoria/ZA

11:40 **Protein photodegradation in the visible range? Mechanistic understanding of protein photooxidation considering traces of photosensitizers**
E. Hipper, Biberach an der Riß/DE , W. Kaiser, Biberach an der Riß/DE, D. Hinderberger, Halle (Saale)/DE, P. Garidel, Biberach an der Riß/DE

LECTURE SCHEDULE

12:00 **Monitoring excited-state relaxation in molecules in live cell**
T. Yang, Jena/DE , A. Chettri, Jena/DE, B. Radwan, Krakow/PL, M. Baranska, Krakow/PL, R. A. Arellano-Reyes, Dublin/IE, T. E. Keyes, Dublin/IE, B. Dietzek-Ivanšić, Jena/DE

yPC-Forum

Digitalisierung – Innovationen in Lehre, Forschung und Industrie

10:40 Uhr, C5a

Digitalisierung ist seit Jahren als eines der großen Zukunftsthemen in aller Munde. Aber wie wirkt sie sich auf unseren Laboralltag oder die Gestaltung von Lehre aus? Wie weit sind Forschungsabläufe jetzt schon digitalisiert und welche Entwicklungen erwarten uns erst noch? Und welches Anforderungsprofil ergibt sich aus einer digitalisierten Industrie für Absolvent:innen?

Im diesjährigen yPC-Forum sprechen wir mit drei Gästen aus Lehre, Forschung und Industrie über den Handlungsbedarf, spannende Innovationen und Zukunftsperspektiven:

- Prof. Dr. Andreas Zumbusch, Advanced Data and Information Literacy Track (ADILT) der Universität Konstanz
- Dr. Wolfgang Wachter, Deutsche Forschungsgemeinschaft
- Dr. Florian Budde, 1. Vorsitzender der Deutschen Bunsen-Gesellschaft und Strategic Advisor, Knowde

Jeder unserer Gäste wird uns seine Perspektive in einem Vortrag vorstellen, wobei es ausreichend Gelegenheit für Fragen aus dem Publikum geben wird. Abschließend werden wir das Thema gemeinsam in einer Podiumsdiskussion interaktiv diskutieren.

yPC-Mitgliederversammlung

12:00-12:30 Uhr, C5a (nur für Mitglieder, members only)

Electrochemistry

C1

10:40 **Keynote Lecture: On the optimization of nitrogen-reduction electrocatalysts**
K. S. Exner, Essen/DE

11:20 **Stability of Supported Single-Crystalline IrO_2(110) Ultrathin Films under Oxygen Evolution Reaction Conditions**
T. Weber, Giessen/DE , V. Vonk, Hamburg/DE, D. Escalera-Lopez, Erlangen/DE, M. J. S. Abb, Giessen/DE, A. Stierle, Hamburg/DE, E. Lundgren, Lund/SE, M. Rohnke, Giessen/DE, S. Cherevko, Erlangen/DE, H. Over, Giessen/DE

11:40 **Tunable Distance of Nanoplatelets in Cadmium Chalcogenide Nanoplatelet Stacks**
R. T. Graf, Hannover/DE , A. Schlosser, Hannover/DE, D. Zámbó, Hannover/DE, J. Schlenkrich, Hannover/DE, P. Rusch, Hannover/DE, A. Chatterjee, Hannover/DE, H. Pfnür, Hannover/DE, N. C. Bigall, Hannover/DE

12:00 **Microscopic Corrosion Studies of RuO_2(110)-TiO_2(110) Model Anodes in the Acidic Water Splitting**
L. Glatthaar, Giessen/DE , T. Weber, Giessen/DE, V. Mohni, Braunschweig/DE, M. J. S. Abb, Giessen/DE, D. Escalera-López, Erlangen/DE, S. Cherevko, Erlangen/DE, H. Over, Giessen/DE

Transport and Storage

C2

10:40 **Flexible, cellulose-based nanocomposite electrodes fabricated via spraying**
M. Betker, Hamburg/DE

11:00 **Fe_2NiO_4/YSZ composite as redox mass for rechargeable oxide batteries (ROBs)**
J. Eigen, Aachen/DE , M. Schroeder, Aachen/DE

11:20 **Protons in mixed-conducting perovskites: Why, how, and how many?**
R. Merkle, Stuttgart/DE , G. Raimondi, Stuttgart/DE, M. F. Hoedl, Stuttgart/DE, J. Maier, Stuttgart/DE

11:40 **Behavior of Salty Methane Co-Clathrates with Monovalent Ions as Guests: An Exploration Based on Molecular Dynamics Simulations**
S. Fritsch, Rostock/DE , D. Paschek, Rostock/DE, R. Ludwig, Rostock/DE

12:00 **Influence of hidden variables on the thermal conductivity of Nanofluids**
J. Tielke, Bremen/DE , B. Schuez, Bremen/DE, M. Avila, Bremen/DE

Catalysis

C103

10:40 **Keynote Lecture: First-Principle Investigation of the Fluorination Reactions in the Simons' Process**
B. Paulus, Berlin/DE , S. Mattsson, Berlin/DE, T. Lindic, Berlin/DE

FRIDAY MORNING Parallel Sessions 2

LECTURE SCHEDULE

Catalysis **C103**

11:20 **Shining light on CO_2 activation over oxide catalysts using transient and operando vibrational spectroscopies combined with DFT**
C. Hess, Darmstadt/DE , J. Weyel, Darmstadt/DE, M. Ziemba, Darmstadt/DE, L. Hofmann, Darmstadt/DE

11:40 **New mechanistic insights into catalytic processes by detection of highly reactive and elusive intermediates**
P. Hemberger, Villigen PSI/CH

12:00 **Water at the Interface with the Photocatalyst Strontium Titanate Viewed by Sum Frequency Generation Spectroscopy**
M. Buessler, Wien/AT , S. Maruyama, Tohoku/JP, H. Onishi, Kobe/JP, E. Backus, Wien/AT

Friday, September 9, 2022, 12:20 - 13:20

12:20 **LUNCH BREAK**

WOMEN'S NETWORKING LUNCH

EXHIBITION OPEN

Friday, September 9, 2022, 13:20 - 14:05

PLENARY LECTURE **C112**

13:20 **Low-Coordination Numbers, Unusual Bonding, and Dispersion Force Effects in Organometallic Complexes**
Philip Power, Davis/US

FRIDAY AFTERNOON Parallel Sessions

Friday, September 9, 2022, 14:10 - 15:30

KEY TOPIC: Dispersion Interactions **C112**

14:10 **Keynote Lecture: Dispersion Interactions in Ion Pair Catalysis and Phosphoramidite Palladium(II) Complexes**
R. M. Gschwind, Regensburg/DE

14:50 **Noncovalent interactions probed by fast magic-angle spinning NMR experiments**
T. Wiegand, Mülheim/DE

15:10 **Phase behavior, hydrogen bonding and ionic mobility in a [3-alkylammonium]$^+$-based protic ionic liquids probed by solid state ^{2}H NMR.**
D. Kolokolov, Novosibirsk/RU , A. E. Khudozhitkov, Novosibirsk/RU, R. Ludwig, Rostock/DE

LECTURE SCHEDULE

Spectroscopy — C5a

14:10 **Ultrafast Backbone Protonation in Channelrhodopsin-1**
T. Stensitzki, Potsdam/DE , S. Adam, Jerusalem/IL, R. Schlesinger, Berlin/DE, I. Schapiro, Jerusalem/IL, K. Heyne, Berlin/DE

14:30 **When Like-charged Ions Attract: Controlling the Size and Distribution of Cation Clusters in Ionic Liquids by Adding Molecular OH-catchers**
J. Busch, Rostock/DE , J. Neumann, Rostock/DE, D. Paschek, Rostock/DE, R. Ludwig, Rostock/DE, T. Youngs, Didcot/GB

14:50 **Dependence of exciton size on solvent character in (6,5)-SWNTs**
M. Elfert, Würzburg/DE , E. Krylov, Würzburg/DE, K. Eckstein, Würzburg/DE, T. Hertel, Würzburg/DE

15:10 **Fabrication of Periodic Spiky Gold Nanoparticle Arrays**
N. Metzkow, Dresden/DE , J. Jia, Evanston/US, T. Odom, Evanston/US

Reaction Kinetics and Dynamics — C5b

14:10 **Keynote Lecture: Decoupling the Role of Atomic Steps and Terraces for the Oxidation of CO on Pd(111) and Pd(332) Surfaces**
D. Borodin, Göttingen/DE , M. Schwarzer, Göttingen/DE, J. Fingerhut, Göttingen/DE, H. Guo, New Mexico/US, T. N. Kitsopoulos, Heraklion/GR, A. M. Wodtke, Göttingen/DE

14:50 **Combining transient IR spectra with DFT to elucidate the active Au sites during CO oxidation on Au/CeO_2(111)**
J. Weyel, Darmstadt/DE , M. Ziemba, Darmstadt/DE, C. Hess, Darmstadt/DE

15:10 **Towards Elementary Rate Constants of Water Formation from the Reaction of Hydrogen and Oxygen on Palladium**
M. Schwarzer, Göttingen/DE , D. Borodin, Göttingen/DE, J. Fingerhut, Göttingen/DE, T. N. Kitsopoulos, Göttingen/DE, A. M. Wodtke, Göttingen/DE

Electrochemistry — C1

14:10 **Galvanophoresis - Highly Efficient Active Colloids Driven by Galvanic Exchange Reactions**
J. Simmchen, Dresden/DE

LECTURE SCHEDULE

FRIDAY AFTERNOON Parallel Sessions

Electrochemistry — C1

14:30 **Modelling Solvation behaviour in highly concentrated Electrolytes**
C. Schwetlick, Ulm/DE , M. Schammer, Ulm/DE, B. Horstmann, Ulm/DE, A. Latz, Ulm/DE

14:50 **Interaction of the Ionic Liquid [C2C1Im][DCA] with Au(111) Electrodes and its Impact on the Electrochemical Stability**
F. Hilpert, Erlangen/DE , J. Yang, Erlangen/DE, Q. Yunsheng, Erlangen/DE, V. Briega-Martos, Erlangen/DE, S. Cherevko, Erlangen/DE, K. Mayrhofer, Erlangen/DE, O. Brummel, Erlangen/DE, J. Libuda, Erlangen/DE

15:10 **Liquid-Liquid and Vapor-Liquid Equilibria of Imidazolium Triflate Ionic Liquids with n-Alkyl Alcohols**
B. Rathke, Bremen/DE , M. Pfeiffer, Bremen/DE, S. Wagenfeld, Bremen/DE, M. Stuckenholz, Bremen/DE, J. Kiefer, Bremen/DE, W. Schröer, Bremen/DE

Transport and Storage — C2

14:10 **Function follows form: Exposed facets determine fundamental properties of colloidal nanocrystals**
C. Klinke, Rostock/DE , M. M. . Ramin Moayed, Hamburg/DE, R. Lesyuk, Rostok/DE, S. Kull, Hamburg/DE, A. Rieckmann, Hamburg/DE, P. Beck, Hamburg/DE, M. Wagstaffe, Hamburg/DE, H. Noei, Hamburg/DE, A. Kornowski, Hamburg/DE, A. B. Hungria, Cadiz/ES, A. Stierle, Hamburg/DE, K. Oldenburg, Rostock/DE

14:30 **Plasmonic charge transfers in metallic and colloidal lattices**
T. A. F. König, Dresden/DE

LECTURE SCHEDULE

Catalysis **C103**

14:10 **Unraveling the Mechanism of the Deacon reaction: CeO_{2-x}(111)/Ru(0001) as model catalyst for the HCl oxidation**
V. Koller, Giessen/DE , A. Spriewald-Luciano, Giessen/DE, S.M. Gericke, Lund/SE, A. Larsson, Lund/SE, C. Sack, Giessen/DE, H. Over, Giessen/DE

14:30 **Adsorption Geometries and Enol-Formation of Butanal on pristine and H-pretreated Pd(111)**
A. Baumann, Kiel/DE , J. Wulfes, Kiel/DE, T. Melchert, Kiel/DE, S. Schauermann, Kiel/DE

14:50 **Tunable Energy Release in Molecular Solar Thermal Systems with Outstanding Reversibility**
O. Brummel, Erlangen/DE , E. Franz, Erlangen/DE, R. Eschenbacher, Erlangen/DE, A. Leng, Erlangen/DE, P. Lorenz, Erlangen/DE, T. Xu, Erlangen/DE, H. Hölzel, Gothenburg/SE, K. Moth-Poulsen, Barcelona/ES, A. Hirsch, Erlangen/DE, J. Libuda, Erlangen/DE

15:10 **Towards resolving structural dynamics in 2D silica and germania films**
L. Gura, Berlin/DE , Z. Yang, Berlin/DE, F. Kalaß, Berlin/DE, M. Brinker, Berlin/DE, H. Junkes, Berlin/DE, W.-D. Schneider, Berlin/DE, M. Heyde, Berlin/DE, H.-J. Freund, Berlin/DE

Friday, September 9, 2022, 15:40 - 16:00

15:40 Poster Awards, Agnes Pockel Award and Closing Session **C112**

POSTER LIST

KEY TOPIC 01: Understanding Dispersion Interactions in Molecular Chemistry

P01 01	**Molecular-Dynamics (MD) simulations of phosphate-/ (bident) iminium-cluster dimers – A question of ion-pairs, H-bonding and dispersion** P. Dullinger, Regensburg/DE, R. Gschwind, Regensburg/DE, D. Horinek, Regensburg/DE, J. Gramüller, Regensburg/DE
P01 03	**Implementing the r²SCAN-3c Composite DFT Method with Slater-Type Orbitals** T. Gasevic, Bonn/DE, M. Bursch, Mühlheim an der Ruhr/DE, J. B. Stückrath, Bonn/DE, S. Grimme, Bonn/DE
P01 04	**A benchmark set of association (free) energies of supramolecular complexes with heavy main group elements** J. Gorges, Bonn/DE, A. Hansen, Bonn/DE, S. Grimme, Bonn/DE
P01 07	**Influence of the PEO-*b*-PHA Block Lengths on the Mesopore Size** L. Q. Wagner, Giessen/DE, F. Breckwoldt, Giessen/DE, B. Smarsly, Giessen/DE
P01 08	**Pnictogens as Dispersion Energy Donors in molecular chemistry** S. Scholz, Chemnitz/DE, A.-M. Fritzsche, Chemnitz/DE, M. Krasowska, Mühlheim/Ruhr/DE, A. A. Auer, Mühlheim/Ruhr/DE, M. Mehring, Chemnitz/DE
P01 09	**Which Computational Methods to Trust for Modelling CO_2 Adsorption on Fe-MOF-74?** W. Schwedland, Berlin/DE, F. Berger, Berlin/DE, F. Müller, Berlin/DE, K. Sillar, Tartu/EE, J. Sauer, Berlin/DE
P01 10	**The Role of Packing, Dispersion, Electrostatics, and Solvation in High-Affinity Complexes of Cucurbit[*n*]urils with Uncharged Polar Guests** F. Biedermann, Karlsruhe/DE, L. Grimm, Karlsruhe/DE, S. Spicher, Bonn/DE, B. Tkachenko, Gießen/DE, P. Schreiner, Gießen/DE
P01 11	**Effect of degree of fluorination on solute-solvent interactions and conformational dynamics of amino acids** P. Imhof, Erlangen/DE, F. Ferraro, Erlangen/DE, H. Razafindrazaka, Erlangen/DE, J. Robalo, Golm/DE, A. Vila Verde, Essen-Duisburg/DE
P01 12	**Synthetic strategies towards binary nanoparticle superlattices and study their optical properties.** S. Kesarwani, Hamburg/DE, H. Lange, Hamburg/DE
P01 13	**Understanding Crystal Packings - Comparing of London Dispersion in Naphthalenediyl-Substituted Dipnictanes** A. Gehlhaar, Essen/DE, E. Schiavo, Mülheim an der Ruhr/DE, A. A. Auer, Mülheim (Ruhr)/DE, S. Schulz, Essen/DE
P01 14	**Substitution effects on the interaction between alpha-hydroxy esters and benzyl alcohol** E. Sennert, Göttingen/DE, M. Lange, Göttingen/DE, M. A. Suhm, Göttingen/DE
P01 15	**H_2 - Halogen benzaldehyde complex studied by rotational spectroscopy** B. Kempken, Göttingen/DE, M. M. Dohmen, Göttingen/DE, P. Pinacho, Hamburg/DE, M. Schnell, Hamburg/DE, D. A. Obenchain, Göttingen/DE

POSTER LIST

KEY TOPIC 01: Understanding Dispersion Interactions in Molecular Chemistry

P01 16	**IR/UV and Raman/UV double resonance spectroscopy for analysis of dispersion interactions in isolated molecular aggregates** P. H. Strebert, Kaiserslautern/DE, D. Bernhard, Kaiserslautern/DE, D. Maue, Kaiserslautern/DE, P. Boden, Kaiserslautern/DE, M. Meta, Kaiserslautern/DE, F. Dietrich, Kaiserslautern/DE, M. Schnell, Hamburg/DE, P. R. Schreiner, Gießen/DE, M. A. Suhm, Göttingen/DE, C. Riehn, Kaiserslautern/DE, M. Gerhards, Kaiserslautern/DE
P01 17	**The Spectroscopic Consequences of Ions Bound inside a Benzo-cryptand Cage** T. S. Zwier, Livermore/US, C. Foley, Livermore/US, C. D. Allen, Livermore/US, P. Ren, Livermore/US
P01 18	**Tuning hydrogen- and host-guest bonding with small molecular changes – self-assembly at the liquid/solid interface investigated by STM** N. Herrmann, Leuven/BE, R. Reynaerts, Leuven/BE, K. S. Mali, Leuven/BE, A. Minoia, Mons/BE, D. De Vos, Leuven/BE, S. De Feyter, Leuven/BE

TOPIC 02: Biophysical Chemistry and Biophotonics

P02 01	**Mapping water thermodynamics in α-Elastin liquid-liquid phase separation** B. König, Bochum/DE, S. Ramos, Bochum/DE, S. Pezzotti, Bochum/DE, M. Havenith, Bochum/DE
P02 02	**Thermophoresis as a promising tool to study ion specificity** S. Mohanakumar, Jülich/DE, S. Wiegand, Jülich/DE
P02 03	**Investigation of the diffusion behaviour of Sr^{2+} in bone marrow** C. Kern, Gießen/DE, A. Pauli, Gießen/DE, R. Jamous, Gießen/DE, T. El Khassawna, Gießen/DE, M. Rohnke, Gießen/DE
P02 04	**Perfusion-Induced Attenuated Total Reflection FTIR Difference Spectroscopy on Membrane Proteins** C. Strothenke, Bielefeld/DE, L. Gött-Zink, Bielefeld/DE, T. Kottke, Bielefeld/DE
P02 05	**Iron oxide as a part of a magnetically directed drug-delivery-system** K. Henze, Dresden/DE, J. Simmchen, Dresden/DE

TOPIC 03: Catalysis

P03 01	**Nanoporous platinum networks gained by a simple synthesis method** L. Möllmann, Oldenburg/DE, M. Osmić, Oldenburg/DE, N. Brinkmann, Oldenburg/DE, K. Al-Shamery, Oldenburg/DE
P03 02	**Adsorption of D_2O and CO on Co_3O_4(111): Water Stabilizes Coadsorbed CO** G. Fickenscher, Erlangen/DE, C. Hohner, Erlangen/DE, T. Xu, Erlangen/DE, J. Libuda, Erlangen/DE
P03 03	**Methanol Conversion on Nanoparticulate Cu/Cu_2O in UHV** M. Grebien, Oldenburg/DE, K. Al-Shamery, Oldenburg/DE
P03 04	**Spectroelectrochemical and IR-photocatalytic investigations of manganese based CO_2-reduction-catalysts** D. Kotwica, Rostock/DE, E. Oberem, Rostock/DE, R. Ludwig, Rostock/DE

POSTER LIST

TOPIC 03: Catalysis

P03 06	**Investigations on the Activation of Amines and Alkenes at Pt(111) Surfaces** N. Brinkmann, Oldenburg/DE, K. Al-Shamery, Oldenburg/DE
P03 07	**Growth and Structures of CoO_x on Pd(100)** J. S. Smyczek, Kiel/DE, M. C. Schmidt, Kiel/DE, P. Hubert, Kiel/DE, S. Schauermann, Kiel/DE
P03 08	**IEDDA/PIRO Reaction as Synthetic Tool for Medium-Sized Carbocycles** J. Ruhl, Giessen/DE, H. A. Wegner, Gießen/DE
P03 09	**Bismuth-based perovskite nanocrystals for photoelectrochemical - photocatalytic applications** R. Altieri, Giessen/DE, M. Wang, Gießen/DE, T. Gatti, Gießen/DE
P03 10	**Influence of the porosity of silica carrier material on the performance of immobilised DMAP in flow catalysis** E. A. Trommer, Giessen/DE, J. S. Schulze, Giessen/DE, B. M. Smarsly, Giessen/DE
P03 11	**Synthesis and Characterization of $Ce_xZr_{1-x-y-z}YyLazO_{2-\delta}$ Oxygen Storage Materials for Application in Three-way Catalysis** E. Prates da Costa, Giessen/DE, U. Goebel, Giessen/DE, A. Hofmann, Giessen/DE, B. M. Smarsly, Giessen/DE
P03 12	**Immobilization of a Peptide-based Catalyst on Mesoporous Silica for Heterogeneous Catalysis** R. D. Brand, Giessen/DE, S. Busche, Berlin/DE, B. M. Smarsly, Giessen/DE, H. G. Börner, Berlin/DE
P03 13	**DFT Investigation of Charged Adsorbents in a Periodic Metallic System – The case of BH_4- Hydrolysis on Ag^0 and Au^0 Nanoparticle Surfaces** B. Raju, Ariel/IL, H. Kornweitz, Ariel/IL, D. Meyerstein, Ariel/IL
P03 15	**Aqueous Photocatalytic Reforming of Methanol in the Liquid and in the Gas Phase over $Pt/SrTiO_3$** M. Deitermann, Bochum/DE, Y. Haver, Bochum/DE, G. W. Busser, Bochum/DE, M. Muhler, Bochum/DE
P03 16	**CdSe quantum dots at ZIF8 hybrid materials for solar hydrogen evolution** L Qian, Jena/DE, M. Wächtler, Jena/DE, B. Dietzek-Ivanšić, Jena/DE
P03 17	**Electrocatalytic studies of dimerizing binuclear Re-complexes using spectroscopic and electrochemical approaches for CO_2 reduction.** V. Caliskanyürek, Braunschweig/DE, M. Obermeier, Berlin/DE, M. Schwalbe, Berlin/DE, S. Tschierlei, Braunschweig/DE

TOPIC 04: Electrochemistry

P04 01	**Tuning the electrochemical stability of norbornadiene-based MOST systems by molecular design** E. Franz, Erlangen/DE, D. Krappmann, Erlangen/DE, L. Fromm, Erlangen/DE, T. Luchs, Erlangen/DE, A. Görling, Erlangen/DE, A. Hirsch, Erlangen/DE, O. Brummel, Erlangen/DE, J. Libuda, Erlangen/DE
P04 02	**Structural Investigations of AuNi-Aerogels** J. Kresse, Dresden/DE, M. Georgi, Dresden/DE, N. Weiß, Dresden/DE, R. Hübner, Dresden/DE, A. Eychmüller, Dresden/DE

POSTER LIST

TOPIC 04: Electrochemistry

P04 03	**Metal Aerogels for Bifunctional Electrocatalysts** C. Wang, Dresden/DE, M. Georgi, Dresden/DE, A. Eychmüller, Dresden/DE
P04 04	**Semiconductor-metal hybrid nanostructures with efficient charge carrier separation** J. Schlenkrich, Hannover/DE, D. Zámbó, Budapest/HU, A. Schlosser, Hannover/DE, M. Rosebrock, Hannover/DE, P. Rusch, Hannover/DE, R. Graf, Hannover/DE, N. Bigall, Hannover/DE, F. Lübkemann, Hannover/DE
P04 05	**Synthesis and Electrochemical Investigation of Boron Verdazyl Radicals** M. Janse van Rensburg, Giessen/DE, S. Kunz, Giessen/DE, D. Schröder, Braunschweig /DE, H. A. Wegner, Giessen/DE
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TOPIC 05: Reaction Kinetics and Dynamics

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P05 03	**Colloidal double semiconductor quantum dots consisting of CdSe and PbS** V. Mittag, Hamburg/DE, M. Dohrmann, Hamburg/DE, L.-F. Mochalski, Hamburg/DE, C. Strewlow, Hamburg/DE, T. Kipp, Hamburg/DE, A. Mews, Hamburg/DE
P05 04	**Photocatalytic Oxidative [2+2] Cycloelimination Reactions with Flavinium Salts: Mechanistic Study and Influence of the Catalyst Structure** N. Archipowa, Manchester/GB, T. Hartman, Prag/CZ, M. Reisnerová, Prag/CZ, J. Chudoba, Prag/CZ, E. Svobodová, Prag/CZ, R. Cibulka, Prag/CZ, R. J. Kutta, Regensburg/DE

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P05 08	**Colloidal CdSe Nanocrystals Deposited into Thin Films and Infiltrated into Nanoporous Matrices for Nonlinear Optical Applications** R. Baruah, Jena/DE, M. Dilshad, Jena/DE, H. N. Gopalakrisha, Jena/DE, V. Korolev, Jena/DE, L. Ghazaryan, Jena/DE, S. Gojare, Jena/DE, A. Szheghalmi, Jena/DE, D. Kartashov, Jena/DE, M. Wächtler, Jena/DE
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P06 02	**HyDRA: inviting theory to predict vibrational spectroscopy data** M. Bödecker, Göttingen/DE, T. L. Fischer, Göttingen/DE, S. M. Schweer, Göttingen/DE, R. A. Mata, Göttingen/DE, M. A. Suhm, Göttingen/DE
P06 03	**In-situ Raman investigations of Ni-based OER electrocatalysts** I. Efthimiopoulos, Düsseldorf/DE, M. Rabe, Düsseldorf/DE
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P06 19	**Setup Of A Spectrometer To Detect Raman Optical Activity** K. Hofmann, Würzburg/DE, T. Preitschopf, Würzburg/DE, I. Fischer, Würzburg/DE
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P06 25	**Infrared reflection absorption spectroscopy (IRRAS) study of organic monolayer reactivity on water surfaces** L. Dittmer, Kiel/DE, J. N. Dühr, Kiel/DE, G Friedrichs, Kiel/DE
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Varrentrappstraße 40-42, 60486 Frankfurt am Main, Germany
Phone: +49 (0)69 7917 363 | geschaeftsstelle@bunsen.de
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