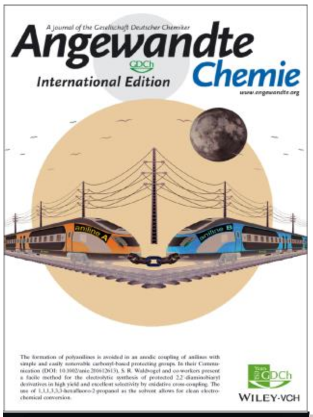
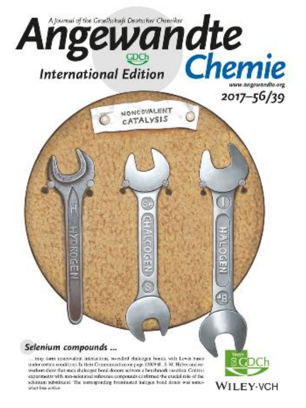
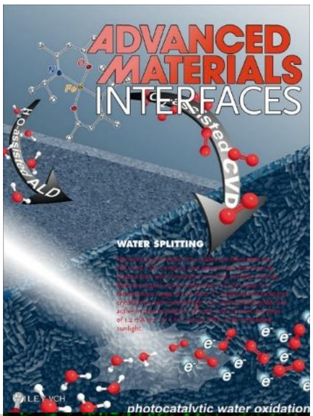
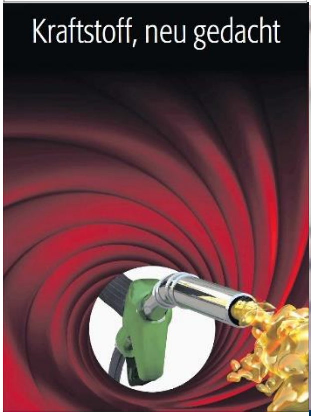
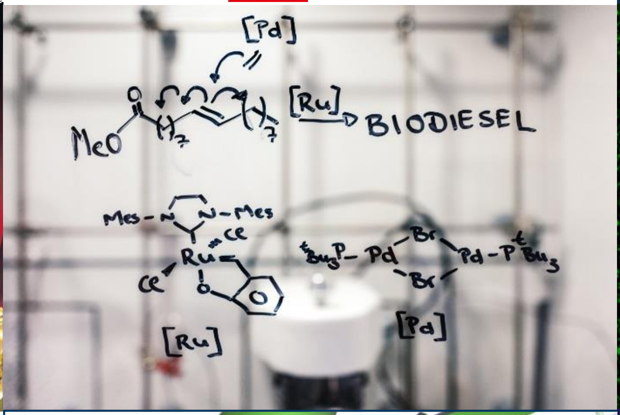
Forschung 2017 – Fakultät für Chemie und Biochemie

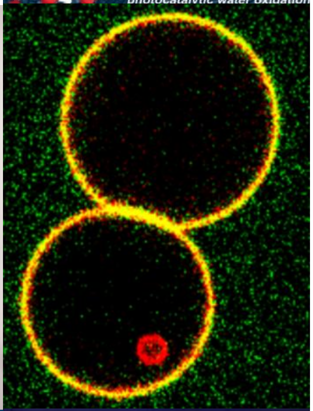


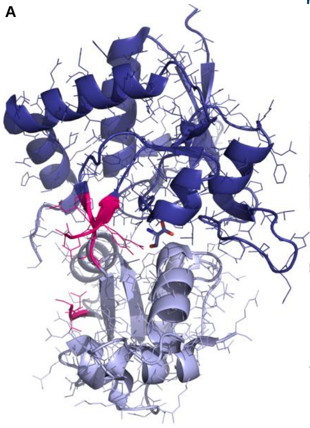


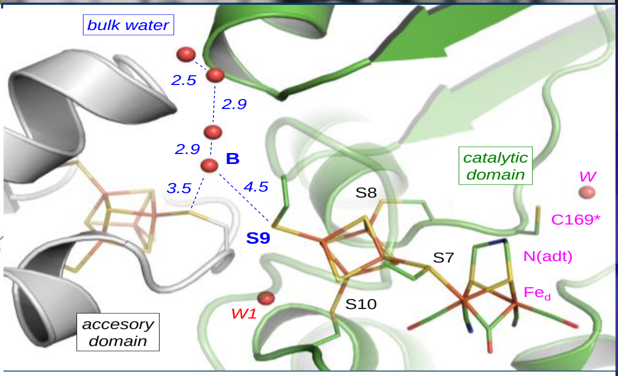


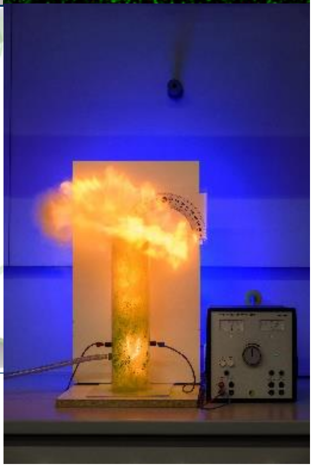


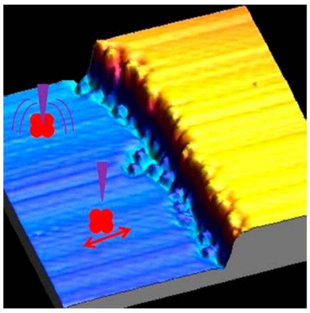


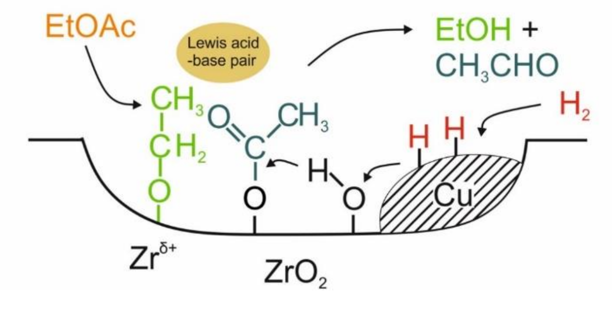


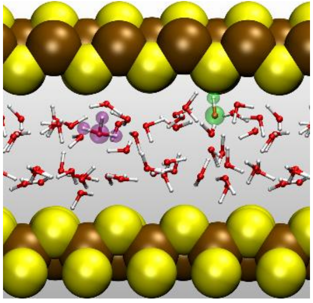












Research 2017 – Faculty of Chemistry and Biochemistry

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Preface

Another year has passed, in which the scientific work groups at the Faculty of Chemistry and Biochemistry of the Ruhr-Universität Bochum have again accomplished a lot. This report highlights the diversity of research performed in the year 2017.

In the tradition of the last years, the report was again organized by the participants of the internship “Introduction to the Scientific Community” (ITSC). The participating master students have been in contact with the principal investigators of the faculty to collect the highlights and edit them into this annual faculty report. This was a valuable experience for all students involved within this project, initiating contact and knowledge exchange between students and researchers. The teamwork of all ITSC participants was excellent and the insights gained into the research of the Faculty of Chemistry and Biochemistry was a very valuable chance.

For more informations on the scientific content of this volume, you are welcome to contact the research groups directly via the links, email-adresses or phone numbers provided in the faculty report.

We hope you enjoy reading.

With the best wishes,

Faculty Report Team of the ITSC internship 2017/18

Kevin Scholten,
Moussa Muhsin,
Faria Huq.

Dear Reader /
sehr geehrte Leserin und Leser,

I am proud to present you the 2017 Edition of the *Research Report* of our Faculty. As in previous years, this report has been compiled and edited by Master students of our Faculty under the *mentorship* of Prof. Nicolas Plumeré as part of their introductory training course "*Introduction to the Scientific Community*". My warmest thanks to them and to all other contributors! The year 2017 has been a very successful one for our Faculty. Our research output is again summarized on more than 15 pages of publications. Moreover, each of our 34 research groups (regardless of status of the PI) presents their "best" paper of the year on one page. Even a quick glance over these *Research Highlight* pages gives you an impression of the amazing diversity and quality of the work that is done in our Faculty. This quality is also reflected in our successes in attracting outside funding, where our Faculty ranks second amongst all Chemistry Departments in Germany in the recent DFG report, and by the fact that we have four ERC grant holders among our colleagues.
My special congratulations go to our 74 PhD graduates from the 2017 year. My best wishes to them, and also to all colleagues and coworkers in our Faculty, as well as to our students.

Enjoy reading!

Ich freue mich, Ihnen hiermit den *Forschungsbericht* unserer Fakultät für das Jahr 2017 präsentieren zu dürfen. Der Bericht ist wie schon in den vorigen Jahren von Studierenden unserer Masterstudiengänge als Teil des Praktikums „*Introduction to the Scientific Community*" zusammengestellt und editiert worden, unter der *mentorship* von Prof. Nicolas Plumeré. Allen Beteiligten ganz herzlichen Dank für ihre Beiträge!
Das Jahr 2017 war wiederum sehr erfolgreich für unsere Fakultät. Sie können sich über ausgewählte Publikationen der einzelnen Arbeitsgruppen informieren, oder sich einfach von den mehr als 15 Seiten Gesamt-Publikationsverzeichnis beeindrucken lassen, die die Vielfalt und die Qualität der Arbeit aller 34 Arbeitsgruppen an unserer Fakultät wiedergeben. Die Fakultät steht mittlerweile deutschlandweit an Platz 2 im Drittmittel-Ranking der DFG, und vier von elf *ERC Grants* an der RUB wurden an Mitglieder unserer Fakultät vergeben.
Meine besonderen Glückwünsche gehen an die 74 Doktorandinnen und Doktoranden, die im Jahr 2017 erfolgreich promoviert haben, zusammen mit meinen besten Wünschen für die Zukunft, die ich auf alle Kolleginnen und Kollegen in den verschiedenen Statusgruppen, und nicht zuletzt auf unsere Studierenden ausdehnen möchte.

Genießen Sie die Lektüre!

N. Metzler-Nolte

Nils Metzler-Nolte
Dekan der Fakultät / Dean of the Faculty

Analytical Chemistry - Analytische Chemie

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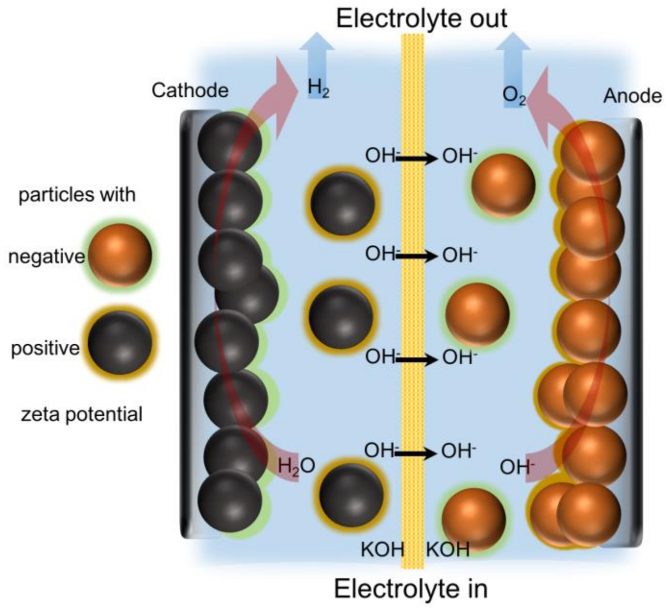
S. Barwe, J. Masa, C. Andronescu, B. Mei, W. Schuhmann, E. Ventosa, *Angew. Chem. Int. Ed.*, **2017**, 56, 8573-8577.

Overcoming the instability of nanoparticle based catalyst films in alkaline electrolyzers by self-assembling and self-healing films.

Despite the increasing reports concerning nanopowders with high electrocatalytic activity for electrochemical water splitting, the fabrication of stable modified electrodes using powder-based catalysts remains a huge challenge. We report an innovation to finally attain very stable catalytic films with self-healing properties using in-situ self-assembly of catalyst particles during the running electrolysis. The catalyst particles are added directly to the electrolyte solution under formation of a suspension that is pumped through a electrolyser cell during operation. Particles with negatively charged surfaces attach on the surface of the anode, while particles with positive surface charges form particle films on the cathode driven by electrostatic forces. These self-assembled catalyst films exhibit self-healing capabilities provided that a sufficient amount of catalyst particles are present in both the anolyte and the catholyte solutions. The proof-of-concept was demonstrated in a non-zero gap alkaline electrolyser using a NiFe layered double hydroxide (LDH) and Ni_xB catalyst nanopowders for anode and cathode, respectively. Steady cell voltages were maintained for at least three weeks during continuous electrolysis at 50-100 mA cm^{-2}.



Schematic representation of an alkaline electrolyzer with self-assembled catalyst films in the presence of suspended catalysts in the electrolyte.

Die Entwicklung stabiler Elektroden für die elektrochemische Wasserspaltung, stellt immer noch – insbesondere hinsichtlich der Elektrodenmodifizierung mittels Nanopartikeln - eine große Herausforderung dar. Ein innovatives Verfahren zur Bildung hochstabiler Katalysatorfilme mit selbstheilenden Eigenschaften wird beschrieben. Das Verfahren basiert auf in-situ selbstassemblierende Nanopartikel, die sich während der Elektrolyse aus einer Suspension, die durch die elektrochemische Zelle gepumpt wird, auf der Elektrodenoberfläche abscheiden. Partikel mit negativ geladener Oberfläche modifizieren die Anode, während Partikel mit positiv geladener Oberfläche sich auf der Kathode abscheiden. Solange sich Katalysatorpartikel im Elektrolyt befinden weisen diese selbstassemblierten Filme einen Selbstheilungseffekt auf. Mittels eines alkalischen Elektrolyseurs konnten unter Verwendung von NiFe-LDH und NixB für die Anoden- bzw. Kathodenseite stabile Zellspannungen bei Stromdichten von 50 bzw. 100 mA cm^{-2} über einen Zeitraum von mindestens drei Wochen beobachtet werden.

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C. Rumancev, A. R. von Gundlach, S. Baier, A. Wittstock, J. Shi, F. Benzi, T. Senkbeil, S. Stuhr, V. M. Garamus, J.-D. Grunwaldt, A. Rosenhahn, *RSC Advances*, **2017**, 7, 45344-45350

Morphological analysis of cerium oxide stabilized nanoporous gold catalysts by soft X-ray ASAXS.

Small angle X-ray scattering (SAXS) is an established method for characterization of biological molecules and systems. SAXS allows structure investigations on the scale from one up to few hundreds nanometers. Anomalous SAXS (ASAXS) examine scattering contrast of different elements containing in the material and allows to determine size and shape of small distributed particles containing different elements in a matrix. Application of ASAXS is especially interesting for catalytic and polymer science**.** Here we applied soft X-ray ASAXS to determine temperature induced structural changes in CeO_2 supported nanoporous gold catalysts. We could show the enhanced thermal stability of gold catalyst after CeO_2 addition and determine the size and shape of gold and CeO_2 particles.

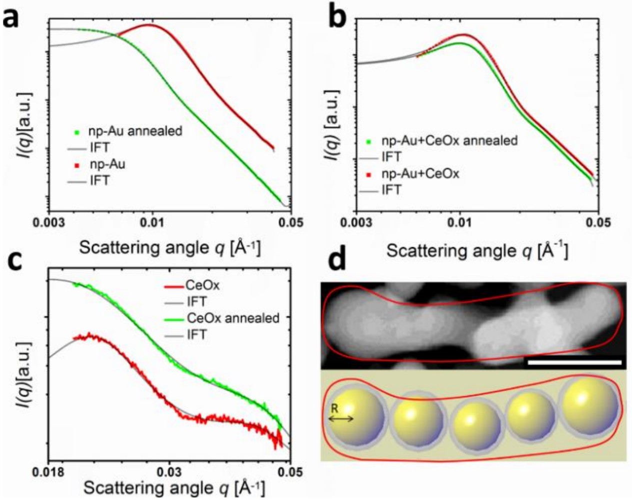

Figure 1: (a) SAXS data of a pure nanoporous gold foam before and after annealing at 520°C. After annealing, as the size of gold particles increases, the peak at 0.01 $Å^{-1}$ is shifted to lower q-values. (b) SAXS data of nanoporous gold foam supported by CeO_2. No major changes are visible before and after annealing (c) The ASAXS data of cerium oxide nanoparticles was obtained after subtraction of scattering curves measured above and below the cerium M-edge (E_1=905eV and E_2=870eV). The data was measured before and after annealing (30 min at 520°C). (d) Transmission electron microscopy image of the pure nanoporous gold foam (scale bar 100 nm) and schematic representation of the model for the foam-like catalyst structure. The 3D gold ligaments were modeled as chains of gold nanoparticles using Indirect Fourier Transformation.

Die Röntgenkleinwinkelstreuung (SAXS) ist eine etablierte Methode um Biomoleküle zu untersuchen. Strukturen in der Größenordnung von einem bis mehreren hundert Nanometer können dabei analysiert werden. Anomales SAXS (ASAXS) nutzt den energieabhängigen Streukontrast unterschiedlicher Elemente in einem Material und erlaubt die elementspezifische Bestimmung von Größen und Formen der vorliegenden Strukturen in einer Matrix. Besonders interessant ist ASAXS im Hinblick auf Anwendungen in der Katalyseforschung und in den Polymerwissenschaften. In dem beschriebenen Experiment haben wir die temperaturinduzierte Strukturveränderung in einem mit CeO_2 Partikeln beladenen Goldkatalysator untersucht. Wir konnten eine erhöhte thermische Stabilität der Strukturen des Katalysators nach der Beladung mit CeO_2 Partikeln zeigen und die Größe und Form der Goldstrukturen sowie der CeO_2 Partikel getrennt bestimmen.

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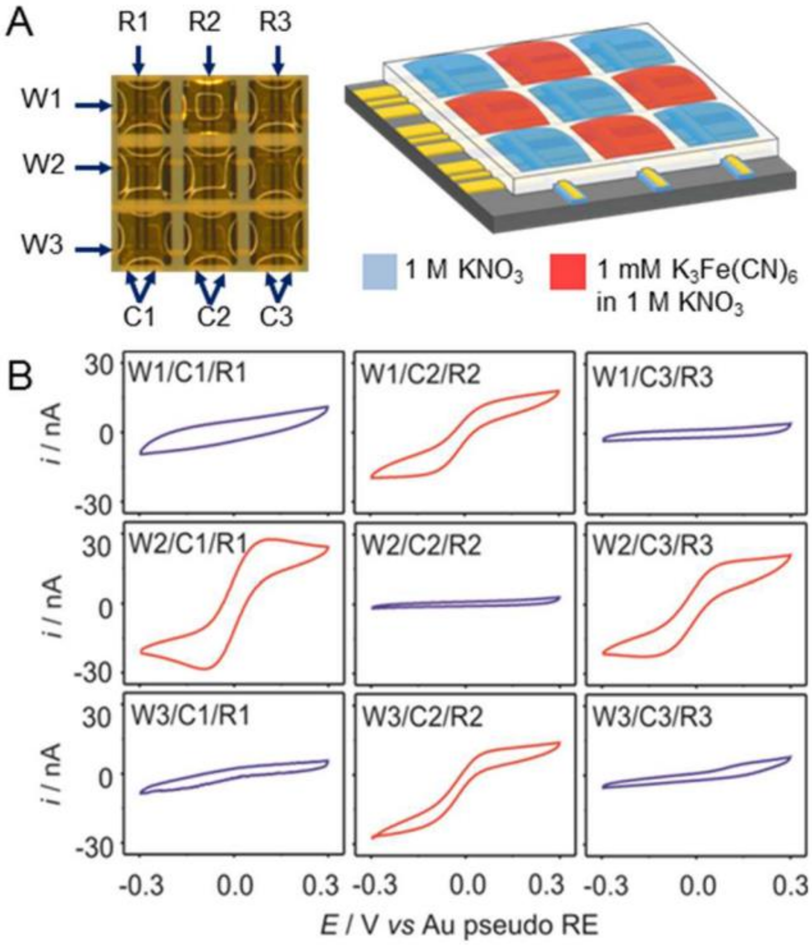
H. Zhang, T. Oellers, W. Feng, T. Abdulazim, E. Saw, A. Ludwig, P. A. Levkin, N. Plumeré
Anal. Chem. **2017**, 89, 5832−5839.

High-Density Droplet Microarray of Individually Addressable Electrochemical Cells

Microarray technology has shown great potential for various types of high-throughput screening applications. The main read-out methods of most microarray platforms, however, are based on optical techniques, limiting the scope of potential applications of such powerful screening technology. Electrochemical methods possess numerous complementary advantages over optical detection methods, including its label-free nature, capability of quantitative monitoring of various reporter molecules, and the ability to not only detect but also address compositions of individual compartments. In this work, we develop a high-density individually addressable electrochemical droplet microarray (eDMA) for the purpose of high-throughput screening. The eDMA allows for the detection of redox-active reporter molecules irrespective of their electrochemical reversibility in individual nanoliter-sized droplets. Orthogonal band microelectrodes are arranged to form at their intersections an array of three-electrode systems for precise control of the applied potential, which enables direct read-out of the current related to analyte detection in spatially separated nanoliter-sized droplets. The eDMA technology opens the possibility to combine the high-throughput biochemical or living cell screenings using the droplet microarray platform with the sequential electrochemical read-out of individual droplets.



Droplet microarray with binary composition containing hexacyanoferrate (red) or electrolyte only (blue). (A) Optical microscope image of 3 × 3 single droplets (600 × 600 μ m, ~ 20 nL each) on the electrode microarray. (B) CVs of 3 × 3 single droplets with hexacyanoferrate and electrolyte arranged alternately.

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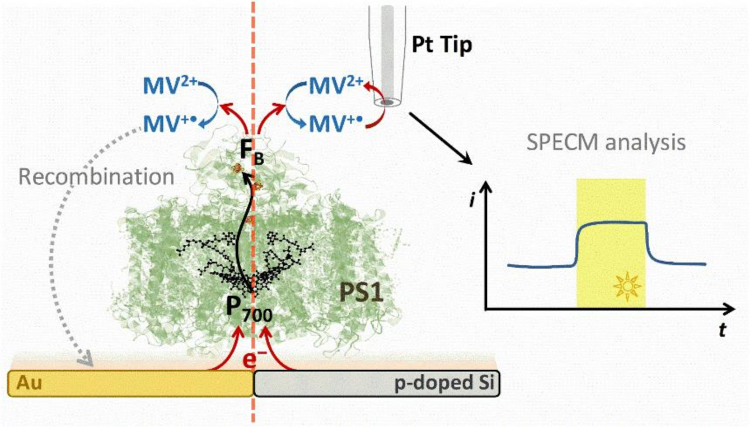
F. Zhao, N. Plumeré, M.M. Nowaczyk, A. Ruff, W. Schuhmann, F. Conzuelo, *Small*, **2017**, 13, 1604093.

Interrogation of a PS1-based photocathode by means of scanning photoelectrochemical microscopy.

Elucidating Charge Recombination Pathways in Photosystem 1 (PS1)-Photocathodes

In the development of photosystem-based energy conversion devices, an in-depth understanding of electron transfer processes involved in photocurrent generation and possible charge recombination is essential as a basis for the development of devices with increased efficiency.

Since charge recombination decreases or cancels out measurable photocurrents, no systematic discrimination between the various possible processes involved in photocurrent generation was possible until now. In our work, a systematic analysis of a PS1-based photocathode demonstrates extensive charge recombination in commonly used gold surfaces while the slower recombination kinetics at a p-doped Si semiconductor enables to visualize concentration profiles of the freely diffusing charge carrier.



Evaluation of biophotoelectrodes with the use of scanning photoelectrochemical microscopy allows the identification of charge recombination and quenching processes by simultaneous monitoring of the photocurrent and associated reduced charge carriers.

Aufklärung von Ladungsrekombinationspfaden in Photosystem 1 (PS1)-Photokathoden

Für die Entwicklung photosystembasierter energieumwandelnder Vorrichtungen mit einer signifikant gesteigerten Effizienz ist ein tiefschürfendes Verständnis der Elektronentransferprozesse, welche in der Photostromgenerierung und Ladungsrekombination beteiligt sind, von essentieller Bedeutung. Da Ladungsrekominationsprozesse verantwortlich für die Verringerung oder gar die gesamte Aufhebung von messbaren Photoströmen sein können, war es bisher nicht möglich eine systematische Diskriminierung zwischen den etwaigen Prozessen, die an der Photostromgenerierung beteiligt sind, zu verfolgen. In unserer vorliegenden Arbeit demonstriert eine systematische Analyse einer PS1-basierten Photokathode extensive Ladungsrekombination, wenn gängig benutzte Goldoberflächen verwendet wurden, während die signifikant geringere Rektionskinetik an einem p-dotierten Si Halbleiter eine Visualisierung der Konzentrationsprofile eines freidiffundierenden Ladungsträgers ermöglicht.

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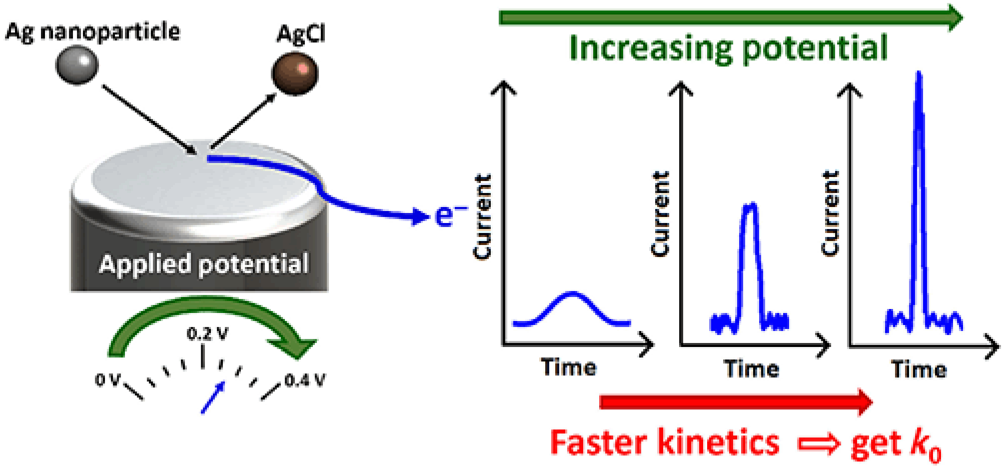
E. Saw, M. Kratz, K. Tschulik, *Nano Research*, **2017**, 10, 3680-3689.

Time-resolved impact electrochemistry for quantitative measurement of single-nanoparticle reaction kinetics

In recent years, nano-impact electrochemistry has been successfully introduced as a new tool to characterize size, agglomeration state, composition and catalytic activity of individual nanoparticles [1,2]. The method employs the stochastic impacts of solution-phase nanoparticles at a potentiostated electrode, for instance to electrochemically oxidize individual particles one by one. Each of these transformative impacts results in a spike in the current transient and the charge transferred in each impact provides the individual particle size.

Here we present that due to the well-defined mass transport at individual particles, not only the charge, but also the duration of individual current spikes contain valuable analytical information that can readily be extracted from nano-impact experiments. Using conventional nano-impact measurements but at high bandwidth, we unravel this information and obtain hitherto inaccessible quantitative insights into nanoparticle reactivity at a single particle scale. This is shown using the oxidation of individual 29 nm diameter silver nanoparticles in four different electrolytes as a proof-of-concept.

Firstly, it is demonstrated that for low overpotentials the peak duration decreases exponentially, that is, the time needed to fully oxidize a single nanoparticle decreases with increasing potential applied at the electrode. Since the charge transferred per impact remains constant, the peak height increases accordingly, as shown in the figure. Secondly, an analytical expression is established that uses the well-defined mass transport at a single dissolving nanoparticle to determine the reaction rate constant from the measured peak duration at a given overpotential. The reaction rate constants for electrochemical oxidation of single silver nanoparticles in four different electrolytes are thus calculated. Thirdly, the peak duration at high overpotentials is found to scale with the concentration of chloride in the electrolyte. Hence, the reaction mechanism of Ag oxidation to form AgCl(s) with chloride diffusion being the mass transport limiting step is identified. Last but not least, it is observed that in the absence of chloride, the peak shape at high overpotentials changes significantly, indicating that the oxidation occurs by formation of $Ag^+(aq)$ and in a step-wise manner.



Time-resolved nanoelectrochemistry is demonstrated as a new tool to determine the reaction kinetics and reaction mechanism at a single nanoparticle.

Inorganic Chemistry I – Anorganische Chemie I

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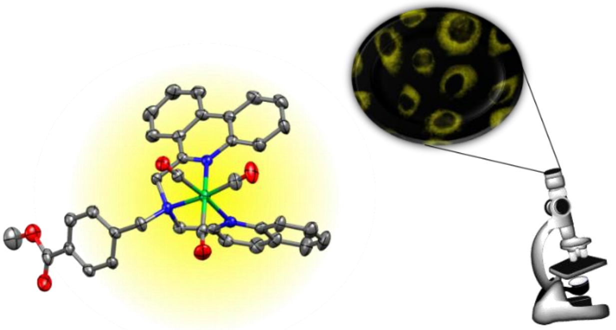
L. J. Raszeja, D. Siegmund, A. L. Cordes, Jörn Güldenhaupt, K. Gerwert, S. Hahn, N. Metzler-Nolte, *Chem. Commun.*, **2017**, 53, 905 – 908.

Asymmetric rhenium tricarbonyl complexes show superior luminescence properties in live cell imaging

Metal complexes often have superior properties for imaging applications. In this paper, the synthesis and photophysical properties of a novel series of rhenium tricarbonyl complexes based on tridentate phenanthridinyl-containing ligands are described. Photophysical data reveal a particularly beneficial luminescence behaviour especially for compounds with an asymmetric ligand set, even in aqueous solutions. The suitability of our new rhenium complexes as potent imaging agents has been confirmed by fluorescence microscopy on living cancer cells, which also confirms superior longtime stability under fluorescence microscopy conditions. Colocalisation studies with commercial organelle stains reveal an accumulation of the complexes in the endoplasmic reticulum for all tested cell lines.



The Figure shows the single crystal X-ray structure of a Re complex that was investigated in this study in depth, as well as its application for imaging in life cells.
Die Abbildung zeigt die mittels Einkristall-Röntgenbeugung bestimmte Struktur eines Re-Komplexes, der in dieser Arbeit für Anwendungen in der zellulären Bildgebung studiert wurde.

Metallkomplexe zeigen oft überlegene Eigenschaften für Anwendungen in der biologischen Bildgebung. In dieser Arbeit berichten wir über die Synthese und Untersuchung der photophysikalischen Eigenschaften einer neuen Serie von Rhenium-tricarbonyl Komplexen mit einem tridentaten Phenanthridinyl-basierten Ligandensatz. Die photophysikalischen Daten zeigen gerade für Verbindungen mit einem unsymmetrischen Ligandensatz ein besonders vielversprechendes Lumineszenzverhalten, sogar in Wasser als Lösemittel. Wir konnten weiter durch Fluoreszenz-Mikroskopie an lebenden Krebszellen zeigen, daß diese vorteilhaften Eigenschaften in der Tat zu überlegener Langzeit-Stabilität unter den Bedingungen der Mikroskopie, und damit zu exzellenten Bildern führen. Kolokalisierungsstudien mit kommerziell erhältlichen Organell-spezifischen Farbstoffen zeigen eine Ansammlung der Komplexe im Endoplasmatischen Reticulum in allen untersuchten Zelllinien.

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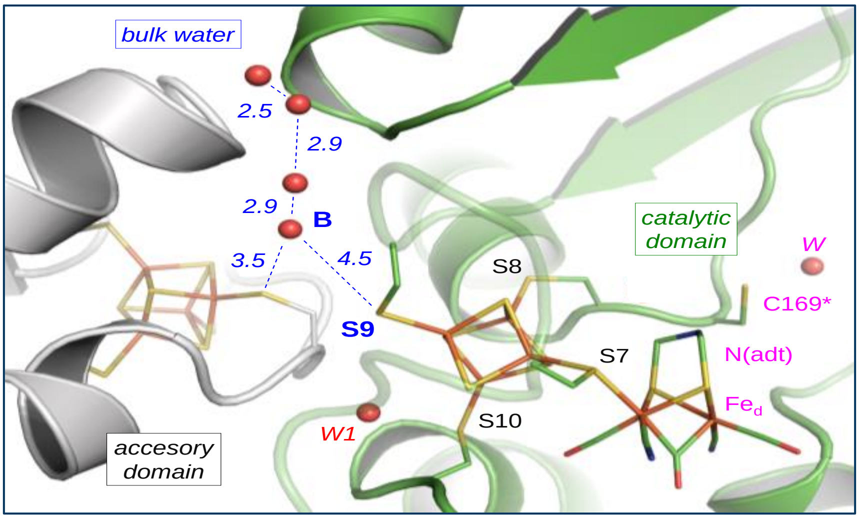
M. Senger, K. Laun, F. Wittkamp, J. Duan, M. Haumann, T. Happe, M. Winkler, U.-P. Apfel, S. T. Stripp, *Angew. Chem. Int. Ed.*, **2017**, 56, 16503-16506.

Reduction of the Catalytic [4Fe-4S] Cluster in [FeFe]-hydrogenases is coupled to Proton Transfer.

In living nature, a variety of chemical reactions take place very slowly. The use of enzymes increases the likelihood or the speed of the catalytic reaction. Especially, the supply and removal of electrons plays a pivotal role for the activation of small molecules (e.g. protons). [FeFe]-hydrogenases are among the most active enzymes to reversibly convert protons to hydrogen gas with unprecedented efficiency. Its active site, the H-cluster, consists of a unique [4Fe4S]-cluster connected to [2Fe$_H$]-site containing an aminodithiolato (adt) ligand that efficiently cycles protons to the low-valent iron center. The molecular details of hydrogen turnover are, however, not yet fully understood.

Using synthetic hydrogenase enzymes, advanced infrared spectroscopy, and electrochemical methods, we could demonstrate that the uptake of an electron at the catalytic center of the enzyme is coupled with the binding of a proton at the [4Fe4S]-cluster. This charge compensation stabilizes the excess electron at the [4Fe4S]-cluster and preserves a conservative configuration of the diiron site. Based on these findings, regulation of the electronic properties in the periphery of metal cofactors seems to be key to orchestrate multi-electron processes at moderate reaction conditions. Thus, this observation has high relevance for understanding the catalytic mechanism of hydrogenases and for the design of synthetic complexes for the production of hydrogen gas.



Putative proton path to the [4Fe-4S] cluster in Clostridium pasteurianum.

The catalytic domain is drawn in green cartoon, the accessory domain is shown in grey. On the right side, relay sites of the adt proton pathway are highlighted (magenta). The sulfur atoms of the ligating cysteines in the catalytic domain are labelled S7 – S10. Four putative water molecules are located in the cleft between catalytic and accessory domains. The most proximal atom may correspond to the base, B. According to our experimental and theoretical data, sulfur atom S9 is protonated in HoxH most likely. Distances are given in Å.

Inorganic Chemistry II – Anorganische Chemie II

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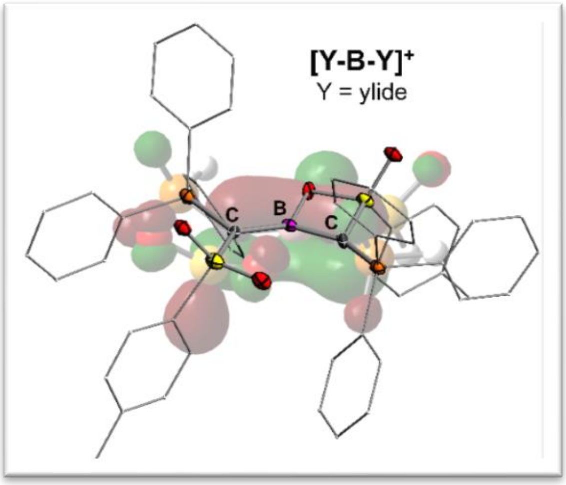
T. Scherpf, K.-S. Feichtner, V. H. Gessner, *Angew. Chem. Int. Ed.* **2017**, 56, 3275-3279.

Using Ylide Functionalization to Stabilize Boron Cations



In the past, the stabilization of reactive compounds by means of an elaborate ligand design has often allowed the isolation of unusual compounds with unique reactivities and fascinating properties. Thereby, strong donor ligands are often required in order to stabilize for example low-valent or electron-deficient compounds. In this publication, we demonstrate that metalated ylides represent a class of so far underdeveloped anionic ligand systems with particularly strong donor properties. The propensity to function as σ- as well as π-donor ligand allows for the electronic stabilization of electron-deficient compounds. This has been shown by means of the isolation of a highly robust ylide functionalized boron cation of type Y-B-Y^+ (Y = ylide). The stability of this system results from a combination of electrostatic interactions as well as π-delocalization within the central C-B-C moiety as shown by DFT calculations. The boron cation reacts with additional Lewis bases to form further boron cations, but undergoes N-H bond activation with primary and secondary amines by addition across the B-C bond.

Die Stabilisierung reaktiver Verbindungen durch geeignetes Ligandendesign hat in der Vergangenheit wiederholt den Zugang zu ungewöhnlichen Verbindungsklassen mit besonderen Reaktivitäten und faszinierenden Eigenschaften ermöglicht. Häufig sind hierbei besonders starke Donorliganden erforderlich, um bspw. die Isolierung niederkoordinierter, elektronenarmer Systeme zu ermöglichen. In dieser Publikation zeigen wir, dass metallierte Ylide eine Klasse bisher kaum erforschter, anionische Liganden mit sehr starkem Donorvermögen darstellen. Ihre Fähigkeit sowohl als σ- als auch als π-Donorligand zu fungieren ermöglicht so die elektronische Stabilisierung elektronenarmer Verbindungen. Dies konnte am Beispiel der Isolierung eines äußerst robusten Ylid-funktionalisierten Borkations Y-B-Y^+ (Y = Ylid) nachgewiesen werden. Die Stabilität in dem System resultiert dabei aus einer Kombination aus elektrostatischen Wechselwirkungen und π-Delokalisierung innerhalb der zentralen C-B-C-Einheit, was mithilfe quantenchemischer Berechnungen belegt werden konnte. Das Borkation ist in der Lage weitere Lewis Basen zu koordinieren und reagiert mit sekundären und primären Aminen unter Aktivierung der N-H-Bindung auf der B-C-Bindung.

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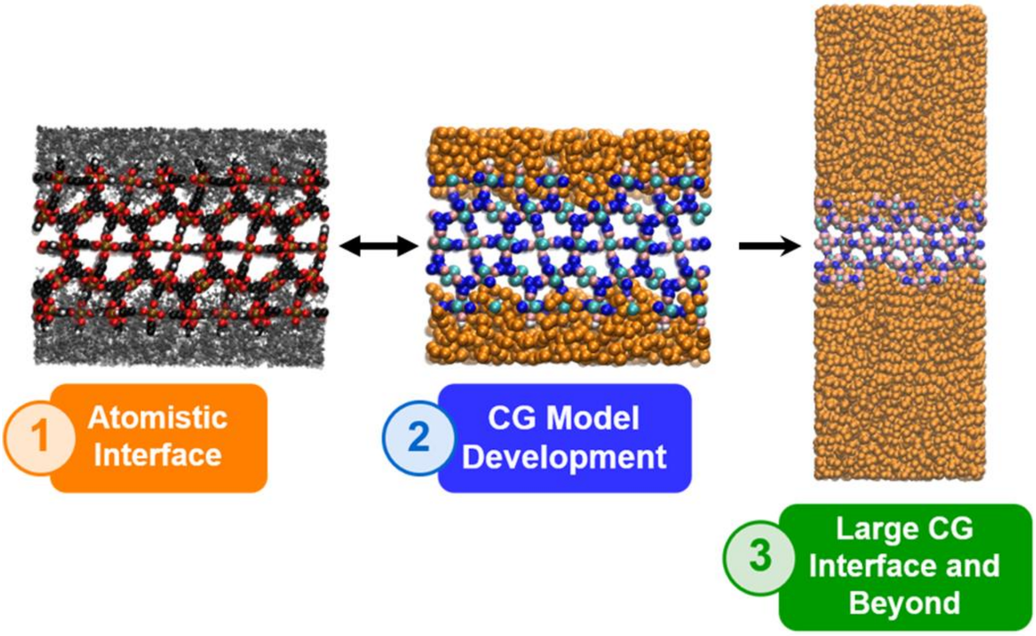
R. Semino, J. P. Dürholt, R. Schmid, G. Maurin. *J. Phys. Chem. C*, **2017**, 121, 21491–21496.

Multiscale Modeling of the HKUST-1/Poly(vinyl alcohol) Interface: From an Atomistic to a Coarse Graining Approach

Metal-organic frameworks (MOFs) have exceptionally large and tunable pore volumes, making them ideal candidates for gas separation applications. However, they are brittle crystalline materials, not suited to make membranes. By embedding them into a polymer matrix in so called mixed matrix membranes, highly efficient and selective separation systems can be made. The main challenge is, however, to understand and control the adhesion of the MOF material to the polymer and the blocking of pores. In this joint publication with the Maurin-group from Montpellier, the novel coarse grained force field model for MOFs, developed in Bochum has been applied to investigate this crucial interface between a polymer and a typical MOF by molecular dynamics investigations. We found that the system can be rather well represented in the coarse grained fashion and could demonstrate to which extent the MOF influences the polymer properties in the bulk.



Metall-organische Netzwerke (MOFs) weisen ausserordentlich große und justierbare Poren auf und sind ideal geeignet für Anwendungen in der Gastrennung. Auf der anderen Seite handelt es sich jedoch um brüchige kristalline Materialien, die sich nicht für Membranen eignen. Durch ihre Einbettung in Polymere in Form sogenannter „mixed matrix membranes“ können jedoch hoch effiziente und selektive Gastrennungs-Systeme erhalten werden. Die Herausforderung besteht nun darin, Verständnis und Kontrolle der Adhäsion des MOFs zum Polymer sowie der möglichen Blockierung der Poren zu erzielen. In dieser gemeinsamen Publikation mit der Maurin-Gruppe in Montpellier wurde das in Bochum neu entwickelte vergröberte Kraftfeld-Modell für MOFs angewendet um diese kritische Grenzfläche zwischen dem Polymer und einem typischen MOF mit Molekulardynamik-Simulationen zur untersuchen. Wir fanden, dass sich das System sehr gut mit dem vergröberten Modell beschreiben lässt und konnten zeigen, wie weit der Einfluss des MOF in die Polymer-Phase hineinreicht.

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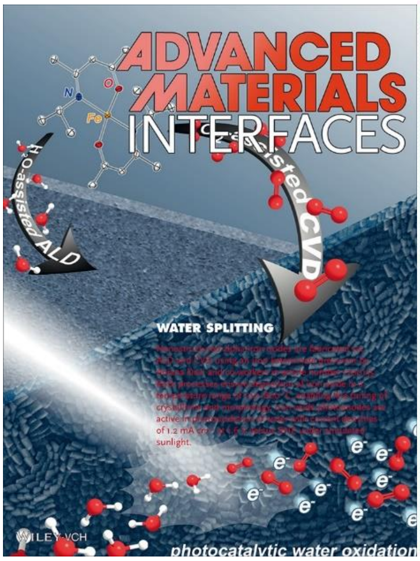
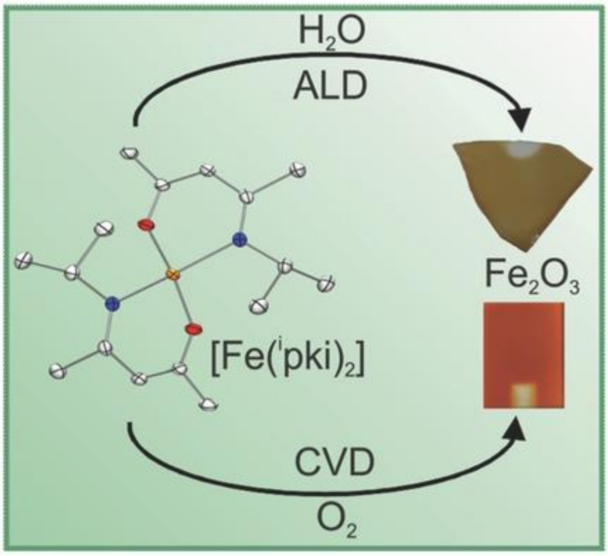
D. Peeters, A. Sadlo, K. Lowjaga, O. Mendoza Reyes, L. Wang, L. Mai, M. Gebhard, D. Rogalla, H.W. Becker, I. Giner, G. Grundmeier, D. Mitoraj, M. Grafen, A. Ostendorf, R. Beranek, A. Devi, *Adv. Mater. Interfaces*, **2017**, 18, 1700155.

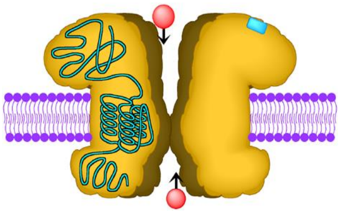
Nanostructured Fe_2O_3 Processing via Water-Assisted ALD and Low-Temperature CVD from a Versatile Iron Ketoiminate Precursor

Vapor phase deposited iron oxide nanostructures are promising for fabrication of solid state chemical sensors, photoelectrodes for solar water splitting, batteries, and logic devices. The deposition of iron oxide via chemical vapor deposition (CVD) or atomic layer deposition (ALD) under mild conditions necessitates a precursor that comprises good volatility, stability, and reactivity. Here, a versatile iron precursor, namely [bis(N-isopropylketoiminate) iron(II)], which possesses ideal characteristics both for low-temperature CVD and water-assisted ALD processes, is reported. The films are thoroughly investigated toward phase, composition, and morphology. As-deposited ALD grown Fe2O3 layers are amorphous, while the CVD process in the presence of oxygen leads to polycrystalline hematite layers. The nanostructured iron oxide grown via CVD consists of nanoplatelets that are appealing for photoelectrochemical applications. Preliminary tests of the photoelectrocatalytic activity of CVD-grown Fe2O3 layers show photocurrent densities up to 0.3 mA cm^{-2} at 1.2 V versus reversible hydrogen electrode (RHE) and 1.2 mA cm−2 at 1.6 V versus RHE under simulated sunlight (1 sun). Surface modification by cobalt oxyhydroxide (Co-Pi) co-catalyst is found to have a highly beneficial effect on photocurrent, leading to maximum monochromatic quantum efficiencies of 10% at 400 nm and 4% at 500 nm at 1.5 V versus RHE.





Biochemistry I – Biochemie I



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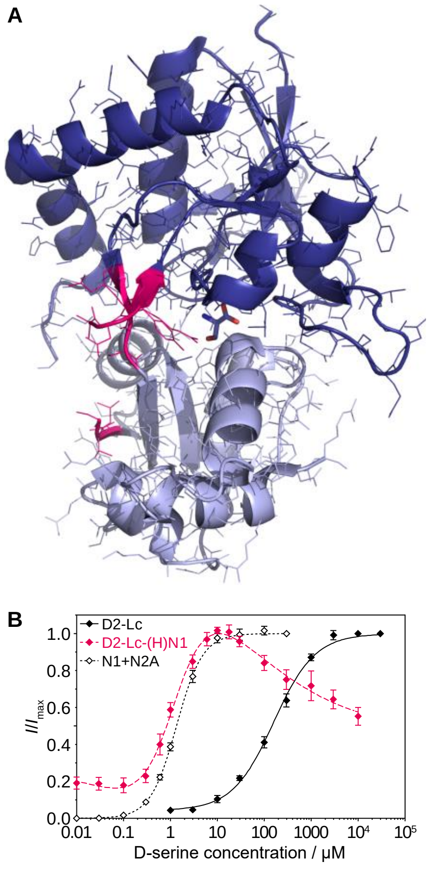
D. Tapken, T.B. Steffensen, R. Leth, L.B. Kristensen, A. Gerbola, M. Gajhede, F.S. Jørgensen, L. Olsen, J.S. Kastrup, *Scientific Reports* **2017**, 7, 46145.

The low binding affinity of D-serine at the ionotropic glutamate receptor GluD2 can be attributed to the hinge region.

Ionotropic glutamate receptors (iGluRs) are ion channels that mediate most of the excitatory signalling in the brain. They are generally activated by the neurotransmitter glutamate, with some additionally requiring glycine or D-serine as a co-agonist that binds to specific subunits. Activation leads to opening of the ion channel, allowing influx of mainly Na^+, in some cases also Ca^{2+} ions. However, one member of the iGluR family, GluD2, has not yet been shown to be activated by any ligand, although it binds glycine and D-serine with low affinity. Using oocyte electrophysiology, isothermal titration calorimetry and molecular dynamics simulations on GluD2 mutants, we investigated why GluD2 binds D-serine with such a low affinity compared to other iGluR subunits. We found that the region of the ligand-binding domain serving as a hinge for the conformational change induced by D-serine binding is responsible for the low affinity. Mutating this hinge to that of the high-affinity D-serine-binding subunit GluN1 strongly increases D-serine affinity of GluD2.



(A) *Structure of the GluD2 ligand-binding domain with bound D-serine (PDB ID 2V3U). The hinge region is highlighted in magenta.* ***(B)*** *GluD2 has low D-serine affinity (solid black line) compared to GluN1 (dotted black line). When mutating its hinge region to that of GluN1, the D-serine affinity of GluD2 increases to that of GluN1 (dashed line in magenta).*

Ionotrope Glutamatrezeptoren (iGluRs) sind Ionenkanäle, die für den Großteil der erregenden Signalweiterleitung im Gehirn verantwortlich sind. Sie werden im allgemeinen durch den Neurotransmitter Glutamat aktiviert, wobei einige zusätzlich Glycin oder D-Serin als Koagonisten benötigen. Die Aktivierung führt zur Öffnung des Ionenkanals, der den Einstrom von Na^+ und in einigen Fällen auch Ca^{2+} ermöglicht. Für ein Mitglied der iGluR-Familie, GluD2, wurde bisher keine Aktivierung durch einen Liganden nachgewiesen, obwohl es Glycin und D-Serin mit geringer Affinität bindet. Mittels Elektrophysiologie an Oozyten, isothermer Titrationskalorimetrie und Molekulardynamiksimulationen haben wir untersucht, warum GluD2 D-Serin mit so geringer Affinität bindet. Wir konnten zeigen, daß die Region der Ligandenbindungsdomäne, die als Gelenk für die Konformationsänderung bei der Bindung von D-Serin dient, für die geringe Affinität verantwortlich ist. Mutiert man dieses Gelenk zu dem der mit hoher Affinität D-Serin bindenden Untereinheit GluN1, erhöht sich die D-Serin-Affinität von GluD2 erheblich.

Biochemistry II - Biochemie II

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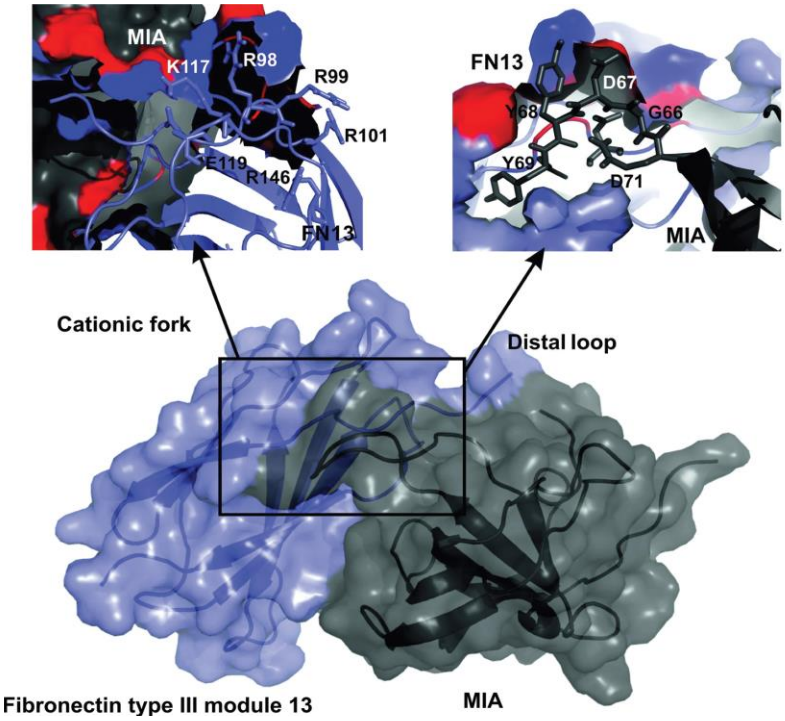
K. T. Yip, X. Y. Zhong, N. Seibel, O. Arnolds, M. Schöpel, R. Stoll, *Biointerphases*, **2017**, 12, 25119.

Human melanoma inhibitory protein binds to the FN12-14 Hep II domain of fibronectin



The heparin binding site (Hep II) of fibronectin plays a major role in tumor cell metastasis. Its interaction with heparan sulfate proteoglycans occurs in a variety of physiological processes including focal adhesion and migration. The melanoma inhibitory activity (MIA) is an important protein that is functionally involved in melanoma development, progression, and tumor cell invasion. After its secretion by malignant melanoma cells, MIA interacts with fibronectin and thereby actively facilitates focal cell detachment from surrounding structures and strongly promotes tumor cell invasion and the formation of metastases. In this report, the authors have determined the molecular basis of the interaction of MIA with the Hep II domain of fibronectin based on nuclear magnetic resonance spectroscopic binding assays. The authors have identified the type III modules 12 to 14 of fibronectin's Hep II as the major MIA binding sites. These results now provide a new target protein-protein binding interface for the discovery of novel antimetastatic agents against malignant melanoma in the future.

Die Heparinbindungsstelle (Hep II) des Fibronektins spielt eine wichtige Rolle bei der Metastasierung von Tumorzellen. Die Wechselwirkung zwischen der Hep II und Proteoglykanen tritt bei verschiedenen physiologischen Prozessen auf, wie z. B. der Zelladhäsion und -migration. Das Melanom-inhibitorische Aktivitätsprotein (MIA) ist funktionell wichtig für die Entwicklung, Progression und die Invasion von Melanomzellen. Das von diesen Zellen sezernierte MIA-Protein wechselwirkt mit dem Fibronektin in der extrazellulären Matrix und ermöglicht dadurch das Ablösen von Tumorzellen und somit deren Invasion. Diese führt letztendlich zur Ausbildung von Metastasen beim malignen Melanom. In dieser Arbeit konnte die molekulare Grundlage der Interaktion zwischen der Hep II-Domäne des Fibronektins und des MIA-Proteins mittels NMR-spektroskopischen Bindungsstudien bestimmt werden. Dabei konnten die Typ III-Module Nr. 12 bis 14 der Hep II-Domäne des Fibronektins als wesentliche Bindungsstelle identifiziert werden. Diese Ergebnisse definieren nun eine neue Protein-Protein-Interaktionsfläche als Zielregion für die zukünftige Entwicklung von Verbindungen gegen die Metastasierung des malignen Melanoms.

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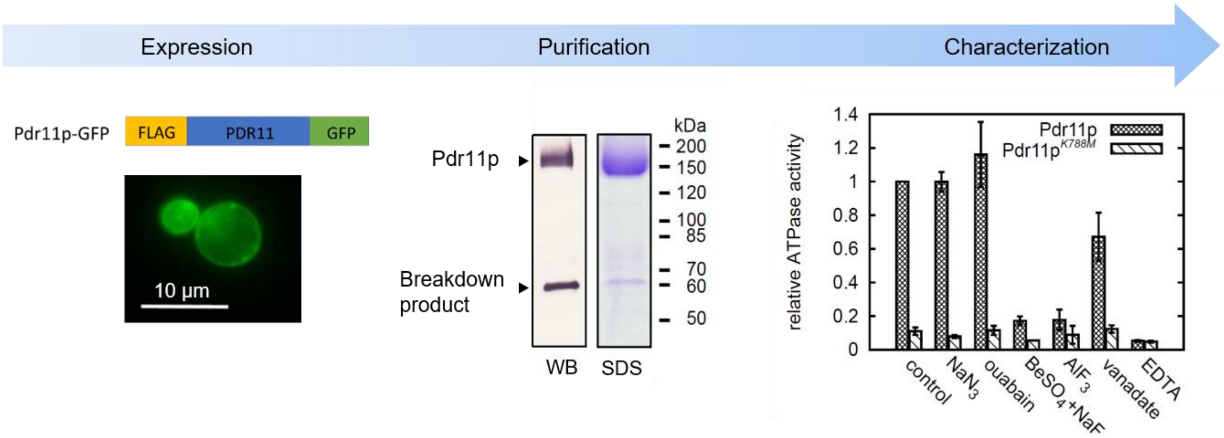
K.R. Laub, M. Marek, L.D. Stanchev, S. Abad Herrera, T. Kanashova, A. Bourmaud, G. Dittmar, T.G. Pomorski. *PLoS One*, **2017**, 12, E0184236.

Purification and characterisation of the yeast plasma membrane ATP binding cassette transporter Pdr11p

Sterols constitute an essential lipid class in eukaryotic membranes whose intracellular levels and distribution are highly regulated. Disorders related to sterol handling in the body cause severe diseases such as atherosclerosis and neurodegeneration. However, the underlying mechanisms are poorly understood. Members of the ATP-binding cassette (ABC) transporter family help controlling the functional compartmentalization of sterols. These energy-powered transporters are proposed to mediate inter- and transbilayer sterol migration. However, direct proof of their function is lacking. This can be attributed to difficulties in handling of integral membrane proteins, their delicacy in production, purification, and characterization of their assembly with membrane lipids. In this study, we describe a purification protocol and the biochemical characterisation of a sterol transporter from yeast. The tools developed within the project will be instrumental to further elucidate the mechanism(s) by which these membrane transporters contribute to sterol uptake.



Sterole sind essentielle Lipidkomponenten in eukaryotischen Membranen, deren intrazelluläre Konzentration und Verteilung stark reguliert werden. Obwohl Störungen im zellulären Steroltransport schwere Krankheiten wie Atherosklerose und eine Degeneration des Nervensystems verursachen, ist über die zu Grunde liegenden molekularen Ursachen nur wenig bekannt. Transportproteine der *ATP-Binding-Cassette* Protein-Superfamilie helfen, die Kompartimentierung von Sterolen zu kontrollieren. Es wird vermutet, dass diese Proteine für den Transport von Sterolen zwischen den beiden Lipidschichten und zwischen verschiedenen Membranen verantwortlich sind. Ein direkter experimenteller Nachweis fehlt jedoch bisher. Das liegt unter anderem daran, dass der Umgang mit integralen Membranproteinen, begonnen bei deren Produktion und Aufreinigung bis hin zu deren Charakterisierung unter Berücksichtigung assoziierter Membranlipide, eine besondere Herausforderung darstellt. In dieser Studie beschreiben wir ein Protokoll zur Aufreinigung und biochemischen Charakterisierung eines Steroltransporters aus der Hefe. Das in diesem Projekt etablierte Protokoll eröffnet neue Möglichkeiten, die molekulare Funktion der Transporter beim Steroltransport aufzuklären.

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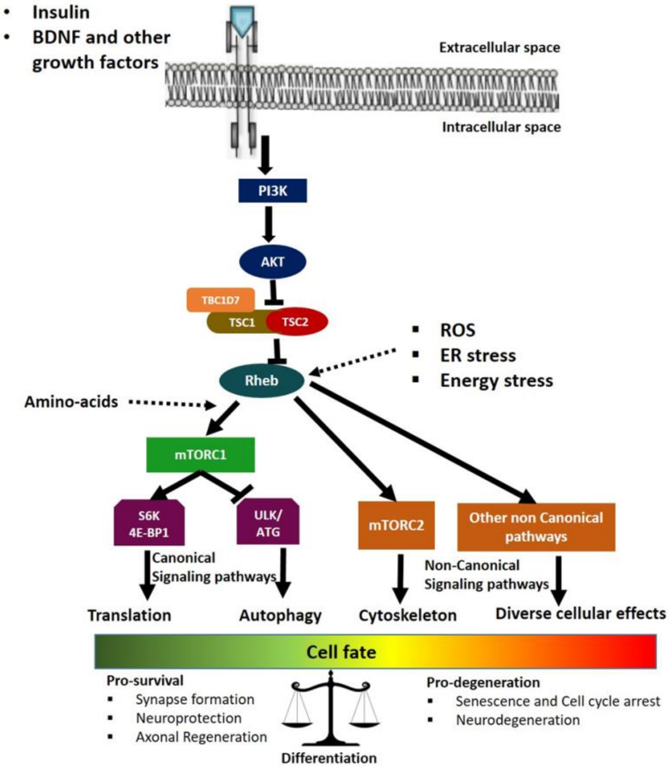
V.N. Potheraveedu, M. Schöpel, R. Stoll, R. Heumann. *Front Neurol.*, **2017**, 8, 264.

Rheb in neuronal degeneration, regeneration, and connectivity

The *Ras homolog enriched in brain* (Rheb) is an intracellular membrane-associated member of the Ras superfamily of GTP-binding proteins. Rheb is involved in the molecular switch regulating cellular growth, cell volume, cell cycle, autophagy, and amino acid uptake mainly via mTOR signaling pathways. We address cell type- and cell state-specific function(s) of Rheb focusing on brain neurons and their surrounding glial cells. In the context of various cellular stress conditions such as oxidative stress, ER-stress, death factor signaling, and cellular aging, Rheb-activation enhances rather than prevents cellular degeneration. This initially unexpected mechanism is discussed in the context of therapy that interferes with Rheb's activity using the antibiotic rapamycin or other newly discovered low molecular weight compounds.



Rheb ist ein Mitglied der membranassoziierten intrazellulären GTP-bindenden Proteinen der Ras-Superfamilie. Rheb steuert -hauptsächlich über den mTOR–Signalweg- zelluläres Wachstum, Zellvolumen, den Zellzyklus, Autophagie und die Aufnahme von Aminosäuren. Wir beschäftigen uns mit den zelltypspezifischen und den vom epigenetischen Zellstatus geprägten Auswirkungen der Rheb Aktivität in Nervenzellen und in den sie umgebenden Gliazellen. Nach zellulärer Stressbehandlung, der durch erhöhten Sauerstoff, durch Apoptose-stimulierenden Faktoren, durch zelluläres Altern und im endoplasmatischen Retikulums verursacht wird, verstärkt Rheb den zellulären Zelltod, statt diesen zu verhindern. Diese überraschende Beobachtung hat Auswirkung auf die Bewertung von therapeutischen Anwendungen, bei der Rheb Aktivität unterdrückt wird, wie dies beim Antibiotikum Rapamycin oder bei neu entdeckten Substanzen mit kleinem Molekulargewicht der Fall ist.

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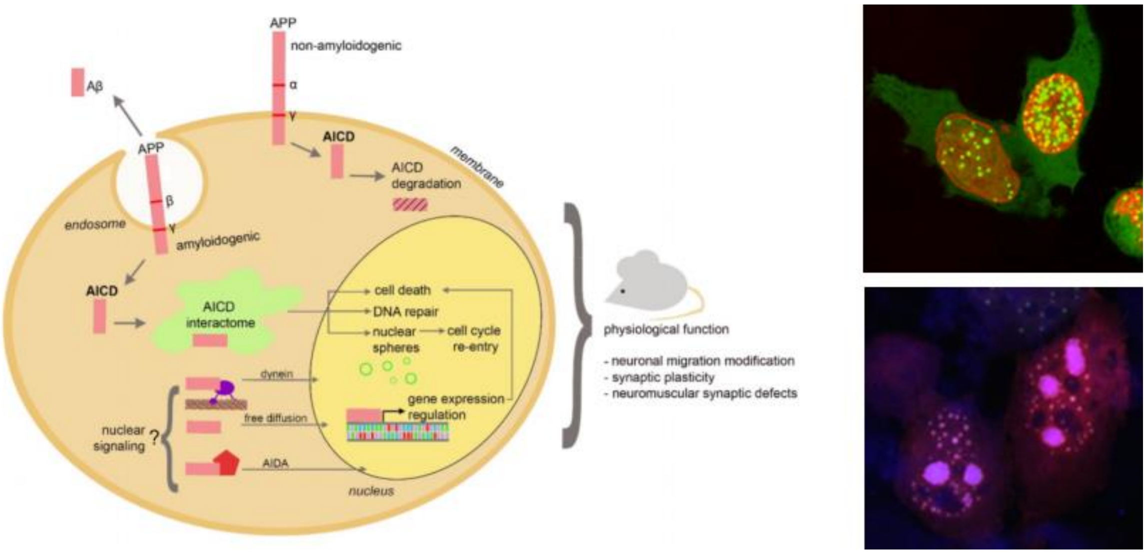
H. Bukhari, A. Glotzbach, K. Kolbe, G. Leonhardt, C. Loosse, T. Müller, *Progress in Neurobiology*, **2017**, 156, 189–213.

Small things matter: Implications of APP intracellular domain AICD nuclear signaling in the progression and pathogenesis of Alzheimer's disease.,

Alzheimer’s disease (AD) is the most common neurodegenerative disease with tens of millions of people affected worldwide. The pathogenesis is still poorly understood and various therapeutical approaches targeting the amyloid β (Aβ) peptide, a product of the amyloidogenic cleavage of the amyloid precursor protein (APP), failed. Moreover, a couple of studies critically questioned the relevance of Aβ in the pathogenesis of AD. Thus, new ideas need to be studied and one highly interesting hypothesis is the APP mediated signal transduction to the nucleus. As a consequence nuclear –potentially toxic- structures emerge, which were recently found to a high extent in human AD tissue and thus, may contribute to neurodegeneration. Relevant for the signaling machinery are modifications at the very C-terminal end of the precursor protein, the APP intracellular domain (AICD). In this year published review we update the knowledge on mechanisms on this small intracellular APP fragment.



Nuclear APP signaling causes generation of spherical aggregates, which might play a role in DNA repair or replication.

Die Alzheimer Erkrankung gehört zu den häufigsten neurodegenerativen Erkrankungen, die Millionen Menschen weltweit betrifft. Die Pathogenese der Erkrankung ist bis heute wenig verstanden und bisherige therapeutische Ansätze mit dem Ziel, das Ausmaß der Amyloid β Peptid Entstehung (ein Produkt der amyloiden APP Prozessierung) bzw. dessen Aggregation zu unterbinden, schlugen fehl. Ein neuartiger Forschungsansatz adressiert die Entstehung von Zellkernaggregaten in Abhängigkeit einer anderen APP Domäne, dem sogenannten AICD (APP intrazelluläre Domäne). Diese potentiell toxischen Kernaggregate konnten jüngst von uns in hohem Ausmaß im Hirngewebe von Alzheimer Patienten gefunden werden. Relevant für die Entstehung dieser Strukturen sind Veränderungen am c-terminalen Ende des APP, die von unserer Arbeitsgruppe untersucht werden. Der in diesem Jahr veröffentlichte Übersichtsartikel gibt ein update über unseren derzeitigen Kenntnisstand zu Mechanismen der APP intrazellulären Domäne.

Organic Chemistry I – Organische Chemie I

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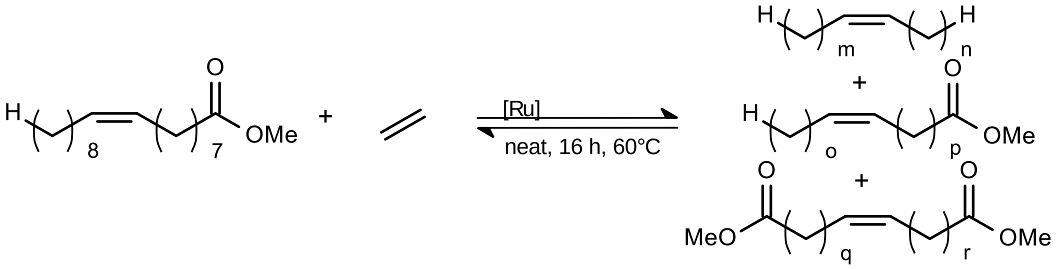
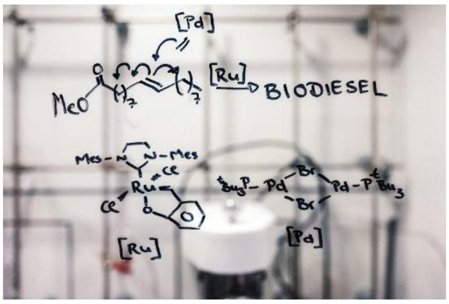
K.F. Pfister, S. Baader, M. Baader, S. Berndt S, L.J. Goossen, *Sci. Adv.*, **2017,** 3, E1602024.

Biofuel by isomerizing metathesis of rapeseed oil esters with (bio) ethylene for use in contemporary diesel engines

In this publication, we disclose an isomerizing olefin metathesis converting rapeseed oil into multi-component blends, consisting of olefins, mono- and dicarboxylates. Until now protocols based on the cross metathesis of rapeseed methyl ester (RME) with short olefins show a good starting point, but the produced biodiesel still does not match the boiling curve of petrodiesel. The developed isomerizing cross-metathesis with (bio)ethylene results in a mixture showing a uniform product distribution with a destillation curve similar to commercial diesel. Unlike the mixtures obtained by non-isomerizing cross-metathesis, they exhibit a more homogeneous distillation curve, making them suitable for use in engines.





Ruthenium catalyzed isomerizing cross-metathesis of rapseed oil esters with (bio)ethylene.

In dieser Publikation präsentieren wir eine isomerisierende Kreuzmetathese zur Umwandlung des erneuerbaren Rohstoffs Rapsöl in ein Mehrkomponentensystem aus Olefinen, Mono- und Dicarboxylaten. Bislang existierende Protokolle, bezogen auf die Kreuzmetathese von Rapsölmethylester mit kurzen Olefinen, zeigen einen guten Ansatzpunkt, jedoch zeigt die Siedekurve des Biodiesels deutliche Unterschiede zu dem des kommerziellen Petrodiesels. Die neu entwickelte isomerisierende Kreuzmetathese mit (Bio)ethen führt zu einem System, welches eine gleichmäßige Produktverteilung mit einer Destillationskurve ähnlich dem kommerziell erhältlichen Petrodiesel zeigt. Entgegen der Systeme erhalten durch nicht-isomerisierender Kreuzmetathese, weist das Biodiesel eine homogene Siedepunktskurve auf, welche das Biodiesel für den Einsatz in Motoren geeignet macht.

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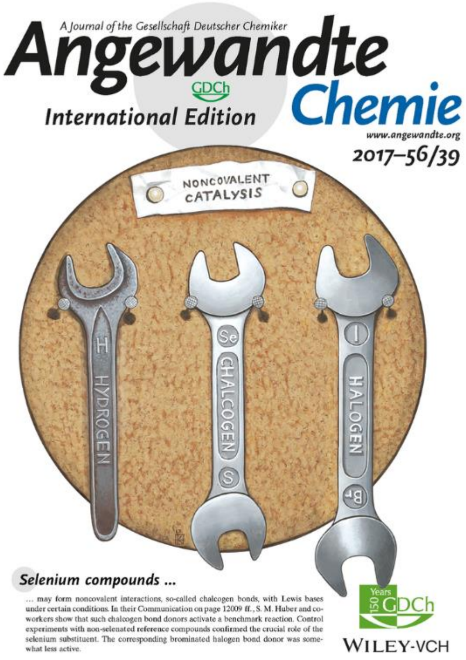
P. Wonner, L. Vogel, M. Düser, L. Gomes, F. Kniep, B. Mallick, D. B. Werz, S. M. Huber,
Angew. Chem. Int. Ed., **2017,** 56, 12009–12012.

Carbon-Halogen Bond Activation by Selenium-Based Chalcogen Bonding



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2017–56/39

Selenium compounds ...

... may form noncovalent interactions, so-called chalcogen bonds, with Lewis bases under certain conditions. In their Communication on page 12009 ff., S. M. Huber and co-workers show that such chalcogen bond donors activate a benchmark reaction. Control experiments with non-selenated reference compounds confirmed the crucial role of the selenium substituent. The corresponding brominated halogen bond donor was somewhat less active.

Chalcogen bonding is a little explored non-covalent interaction similar to halogen bonding. This manuscript describes the first application of selenium-based chalcogen bond donors as Lewis acids in organic synthesis. To this end, the solvolysis of benzhydryl bromide served as a halide-abstraction benchmark reaction. Chalcogen bond donors based on a bis(benzimidazolium) core provided rate accelerations versus background reactivity in the order of 20-30. Several comparison experiments provide clear indications that chalcogen bonding is the origin of the observed activation. The performance of the chalcogen bond donors is superior to that of the related brominated halogen bond donor.

Chalkogenbrücken sind bisher wenig erforschte nicht-kovalente Wechselwirkungen, welche vergleichbar mit Halogenbrücken sind. Diese Arbeit beschreibt die erste Anwendung selen-basierter Chalkogenbrückendonoren als Lewissäuren in der organischen Synthese. Als Testreaktion zur Halogenidabstraktion diente die Solvolyse von Benzylhydrylbromid. Chalkogen¬brückendonoren, welche auf einem Bis(benzimidazolium)-Grund¬gerüst basieren, ergaben Reaktionsbeschleunigungen in einer Größenordnung von 20-30 im Vergleich zur Hintergrundreaktion. Mehrere Vergleichsexperimente lieferten klare Hinweise darauf, dass die beobachtete Aktivierung auf Chalkogenbrücken zurückgeführt werden kann. Zudem sind die eingesetzten Chalkogenbrückendonoren dem entsprechenden bromierten Halogenbrückendonor in ihrer Aktivität überlegen.

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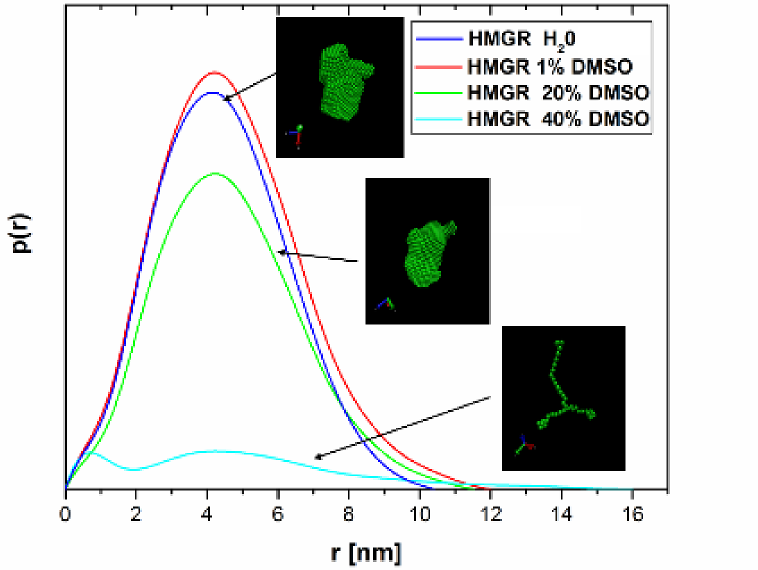
M. Dirkmann, J. Iglesias-Fernández, V. Muñoz, P. Sokkar, C. Rumancev, A. von Gundlach,
O. Krenczyk, T. Vöpel, J. Nowack, M. A. Schroer, S. Ebbinghaus, C. Herrmann,
A. Rosenhahn, E. Sanchez-Garcia, F. Schulz, *ChemBioChem*, **2017**, 19, 153-158.

A Multiperspective Approach to Solvent Regulation of Enzymatic Activity: HMG-CoA Reductase

White biotechnology is a rapidly growing field in industrial catalysis in which enzymes are employed as highly selective catalysts for a variety of chemical reactions. To this end, the enzymes often must function under non-natural solvent conditions to ensure high substrate solubility. In many cases, organic (co-)solvents accelerate the denaturation of the enzymes and the underlying mechanisms for this behavior are poorly understood. In this paper, we show a multi-perspective investigation of the interactions between the HMG-CoA-reductase from the thermoacidophile archaeon *Sulfolobus solfataricus* and different co-solvents in an aqueous buffer. Enzyme kinetics, calorimetrics, fluorescence spectroscopy, small-angle x-ray scattering and molecular dynamics simulations reveal the solvent-specific interaction patterns and give hints on as to how the activity and structural integrity of the tetrameric enzyme is affected. This includes not only a decrease but also an increase of activity in several instances.



Small-angle x-ray scattering reveals the structural alteration of the enzyme at increasing DMSO concentrations.

Die Weiße Biotechnology ist ein rasch wachsendes Feld der industriellen Katalyse und nutzt Enzyme als hochselektive Katalysatoren für zahlreiche Synthesen. In diesem Kontext müssen die Enzyme oftmals in Solvensgemischen eingesetzt werden, welche die Löslichkeit der Substrate sicherstellen sollen. Lösemittel führen jedoch nicht selten zu nur unzureichend verstandenen Aktivitätsverlusten der Enzyme. In diesem Artikel beschreiben wir die Untersuchung der Interaktionen zwischen der HMG-CoA-Reduktase aus dem thermoacidophilen Archaeon *Sulfolobus solfataricus* und verschiedenen Lösemittelgemischen. Enzymkinetik, Kalorimetrie, Fluoreszenzspektroskopie, Röntgenkleinwinkelstreuung und Molekulardynamik-Simulationen werden kombiniert, um die lösemittelspezifischen Wechselwirkungen zu beleuchten.

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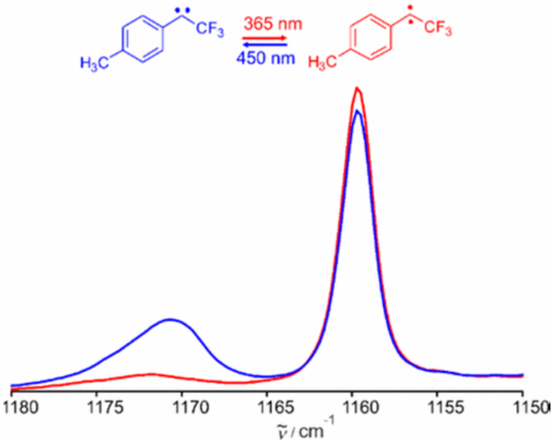
Y.A. Tsegaw, P.E. Kadam, N. Tötsch, E. Sanchez-Garcia, W. Sander, *J. Am. Chem. Soc.* **2017**, 139, 12310-12316.

Is Magnetically Bistabillity of Carbenes a General Phenomenon? Isolation of a Simple Aryl(trifluoromethyl)carbenes in Both Their Singlet and Triplet States

The general belief is that carbenes are isolated in low-temperature matrices in their ground spin states, either singlet or triplet depending on the nature of the carbene. Nevertheless, a few carbenes are reported to change their spin state at cryogenic temperatures upon irradiation with light. In our study, *p*-Tolyl(trifluoromethyl)carbene and the related fluorenyl-(trifluoromethyl)carbene can be generated in both their triplet and singlet states, and both states coexist under the conditions of matrix isolation. According to our calculations, the singlet and triplet states of these carbenes are energetically nearly degenerate. The spin state can be changed by warming up the matrix or using light of different wavelength. An alternative way to generate the singlet carbene is a hydrogen-bonded complex with water. Our studies show that magnetic bistabillity of carbenes is a general phenomenon that only depends on the singlet-triplet gap of the carbene. This opens the way for the development of new optically switchable magnetic materials.



Switching of singlet and triplet states.

Allgemein wird geglaubt, dass Carbene in Matrices bei tiefen Temperaturen in ihrem Grundzustand isoliert werden, entweder als Triplett oder Singulett, je nach der Art des Carbens. Trotzdem finden sich in der Literatur Carbene, die ihren Spinzustand bei kryogenen Temperaturen durch Bestrahlung mit Licht wechseln können. In unserer Studie konnten *p*-Tolyl(trifluoromethyl)carben und das verwandte fluorenyl-(trifluoromethyl)carben sowohl im Singulett- als auch im Triplettzustand erzeugt warden, und beide Spinzustände existieren gleichzeitig unter Matrixbedingungen. Nach unseren Rechnungen sind Singulett und Triplettzustand dieser Carbene fast entartet. Der Spinzustand kann durch aufwärmen der Matrix oder durch Belichtung der Matrix mit Licht unterschiedlicher Wellenlängen gewechselt werden. Eine alternativer Weg zur Erzeugung des Singulett Carbenes ist ein wasserstoffverbrückter Komplex mit Wasser. Unsere Untersuchungen zeigen, dass magnetische Bistabilität von Carbenen ein allgemeines Phänomen ist und nur vom Energieunterschied zwischen Singulett-und Triplett Zustand abhängt. Dies eröffnet einen neuen Weg zur Entwicklung von optisch schaltbaren magnetischen Materialien.

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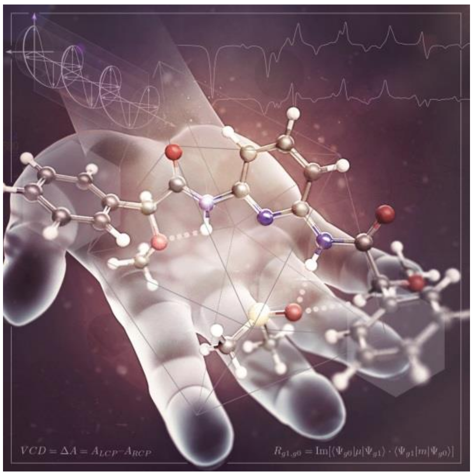
D.P. Demarque, C. Merten, *Chem. Eur. J.*, **2017**, 23**,** 17915–17922.

Intra- vs. intermolecular hydrogen bonding: Solvent-dependent conformational preferences of a common supramolecular binding motif from 1H-NMR and VCD spectra.

When predicting binding properties of small molecules or larger supramolecular aggregates, intra- and intermolecular hydrogen bonds are often considered the most important factor. Spectroscopic techniques such as ^{1}H-NMR spectroscopy are typically utilized to characterize such binding events, but interpretation is often qualitative and follows chemical intuition. In this study, we compare the effects of solvation on the intramolecular hydrogen bonding of two chiral 2,6-pyridinediyl-dialkylamides. In comparison with ^{1}H-NMR spectroscopy, vibrational circular dichroism (VCD) spectroscopy proved to be more sensitive to conformational changes. The change of the solvent from $CDCl_3$ to DMSO-d_6 generates mirror-image VCD spectra for the same enantiomer – something that should only happen when the opposite enantiomer is measured. The detailed analysis of the VCD spectra shows that the common sense of the sterically less hindered group being more prone to solvation does not hold. Clearly, there is a competition between intra- and intermolecular hydrogen bonding and we show that in the asymmetrically substituted compound both amide hydrogens are equally likely to be solvated.



In der qualitativen Vorhersage der intermolekularen Wechselwirkungen kleiner Moleküle oder supramolekularer Aggregate werden Wasserstoffbrückenbindungen meist als wichtigster Parameter herangezogen. Spektroskopische Techniken wie ^{1}H-NMR Spektroskopie sind dabei typische Charakterisierungsmethoden für solche Bindungen, aber die Interpretation der Spektren ist oft qualitative und meist basierend auf chemischer Intuition. In der vorliegenden Arbeit haben wir den Effekt von Solvatation auf die intramolekularen Wechselwirkungen zweier chiraler 2,6-Pyridinediyldialkylamide untersucht. Im Vergleich mit ^{1}H-NMR Spektroskopie hat sich der Schwingungszirkulardichroismus (VCD) als deutlicher empfindlicher für Konformationsveränderungen dargestellt. Ein Lösungsmittelwechsel von $CDCl_3$ zu DMSO-d_6 hat sogar zu einer Spiegelung der VCD Spektren desselben Enantiomers geführt, was normalerweise nur für Enantiomerenpaare beobachtet wird. Die Analyse der VCD Spektren zeigt schließlich, dass der intuitive Ansatz der bevorzugten Solvatation der sterisch weniger gehinderten Gruppe hier nicht greift. Im Gegenteil, die Konkurrenz zwischen intra- und intermolekularen Wasserstoffbrücken führt im asymmetrisch substituierten Diamid zu einer gleichmäßigen Solvatation beider Amid-Protonen.

Physical Chemistry I – Physikalische Chemie I

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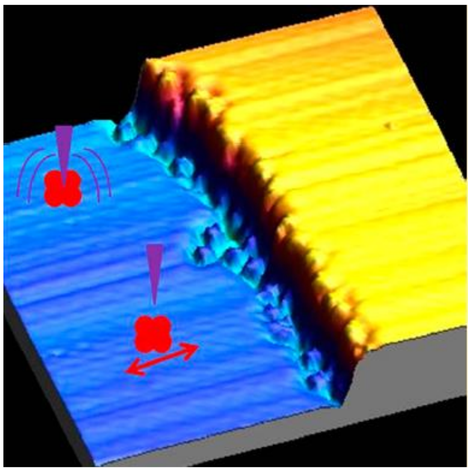
G. Antczak, K. Boom, and K. Morgenstern, *J. Phys. Chem. C.*, **2017**, 121, 542-549.

Revealing the Presence of Mobile Molecules on the Surface

Mobile molecules crossing freely underneath the scanning tip of a scanning tunneling microscope create a uniform diffusive noise, making the identification of single molecules on the surface a challenge. We demonstrate the possibility of detecting mobile molecules on a surface by scanning tunneling microscopy and reveal how the diffusive noise is created. Additionally, we show that a molecule caught in the tip−sample junction allows us to explore the potential energy surface of the system. Finally, voltage pulses disturb the mobile molecules, causing the loss of that ability. They also allow the creation of islands on the surface. Most of the investigations were done for Co- and Cu-phthalocyanine (Pc) on Ag(100). However, the concept is limited to neither Pc molecules nor Ag(100), as shown for a different organic molecule, astraphloxin, on Cu(111).



STM image of Ag(100) surface with Cu-PC molecules close to a step edge. At the lower side of the edge (in blue) and the upper step edge (in yellow) individual molecules are visible. On the terraces a diffusive noise indicates that the molecules follow the tip's field during scanning as sketched.

Wenn Moleküle erheblich schneller auf einer Oberfläche diffundieren, als sich die Aufnahmespitze eines Rastertunnelmikroskops über diese Oberfläche bewegt, dann erzeugen sie durch häufige Unterkreuzung unter der Spitze ein gleichmäßiges Rauschen. In dem Artikel zeigen wir anhand der Moleküle Co- und Cu-Phtalocyanin auf Ag(100) und Astraphloxin auf Cu(111), wie diese mobile Moleküle dennoch detektiert werden können und untersuchen die genaue Ursache des gemessenen Rauschens. Außerdem können einzelne Moleküle durch das Feld der Spitze eingefangen werden. Durch das Ziehen dieser Moleküle über die Oberfläche kann die Potentialenergiefläche des Systems abgebildet werden. Noch höhere Felder in Form einzelner Spannungspulse können die diffundierenden Moleküle derart verändern, dass sie in Inseln immobilisiert werden. Dies dient dem direkten Nachweis Existenz der Moleküle.

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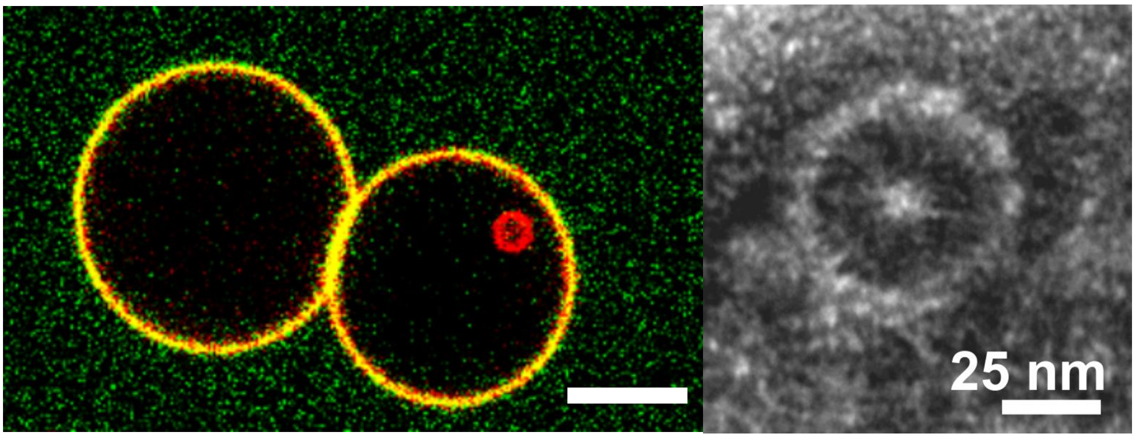
Nucleotide-dependent farnesyl switch orchestrates polymerization and membrane binding of *human* guanylate-binding protein 1.

Guanylate binding proteins represent important players of innate immunity and their biosynthesis is strongly induced upon interferon stimulation. We show that the farnesyl tail at the C-terminus of *human* guanylate binding protein 1 (*h*GBP1) is reponsible for membrane anchorage but that only GTP binding to *h*GBP1 leads to the release of the farnesyl tail triggering membrane binding. Subsequently, GTP hydrolysis catalyzed by *h*GBP1 evokes tethering of lipid membrane vesicles. Alternatively, *h*GBP1 may form ordered, ring-like structures which grow further to form elongated rods but only under the prerequisite of both farnesylation of the enzyme and the availabilty of GTP. The major structural changes of the protein producing force and the enzymatic activity are intimately coupled to each other.



In the presence of GTP farnesylated human GBP1 binds to lipid membranes and leads to tethering of the vesicles shown by fluorescence microscopy in the left hand panel (scale bar 5 µm). In the presence of GTP with no membrane present GBP1 forms ring like supramolecular structures with the farnesyl tails located in the center observed in the electron micrograph.

Die Vertreter der Klasse *humaner* Guanylat bindender Proteine (*h*GBP) sind Bestandteile der immanenten Immunabwehr. In dieser Publikation, die zusammen mit Kollegen aus Genf, Erlangen, Köln und Langen erarbeitet wurde, beschreiben wir molekulare Details der Funktionsweise dieser Proteine. *h*GBP1 verfügt über einen Lipidanker (eine endständige Farnesylgruppe), der erst bei Bindung des Cofaktors Guanosintriphosphat (GTP) "ausgefahren" wird und zur Membranverankerung führt. Alternativ dazu bildet das Protein geordnete Polymere (s. elektronenmikroskopische Aufnahme in der Abbildung), die sich unter GTP Hydrolyse zunächst als ringförmige und im weiteren Verlauf als röhrenförmige Strukturen ausbilden. Kinetische Analysen der Enzymaktivität zeigen, dass die katalytische Aktivität und die damit verbundenen Strukturänderungen des Proteins bei den genannten Vorgängen unterschiedliche Phasen durchlaufen und eine Kopplung von enzymatischer GTP Hydrolyse und mechanischer Arbeit aufweisen.

Physical Chemistry II – Physikalische Chemie II

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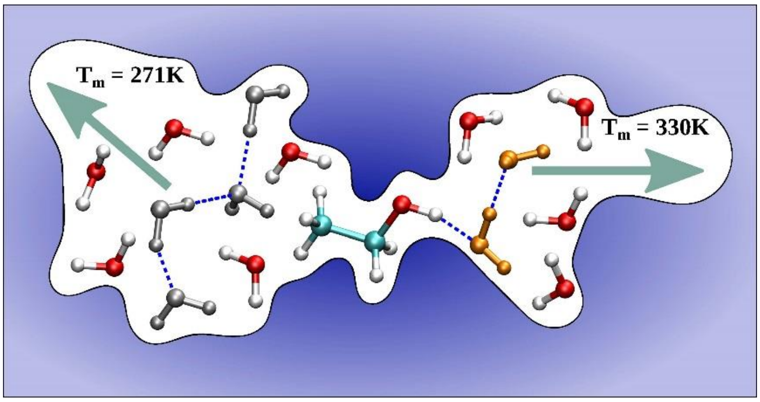
F. Böhm, G. Schwaab, M. Havenith, *Angew. Chem.*, **2017**, 56 (33), 9981–9985

Mapping hydration water around alcohol chains by THz calorimetry

THz spectroscopy was used to probe changes that occur in the dynamics of the hydrogen bond network upon solvation of alcohol chains. The THz spectra can be decomposed into the spectrum of bulk water, tetrahedral hydration water, and more disordered (or interstitial) hydration water. The tetrahedrally ordered hydration water exhibits a band at 195 cm^{-1} and is localized around the hydrophobic moiety of the alcohol. The interstitial component yields a band at 164 cm^{-1}, which is associated with hydration water in the first hydration shell. These temperature-dependent changes in the low-frequency spectrum of solvated alcohol chains can be correlated with changes of heat capacity, entropy, and free energy upon solvation. Surprisingly, not the tetrahedrally ordered component but the interstitial hydration water is found to be mainly responsible for the temperature-dependent change in ΔC_p and ΔG. The solute-specific offset in free energy is attributed to void formation and scales linearly with the chain length.



Änderungen im Wasserstoffbrückennetzwerk von in Wasser gelösten Alkoholketten wurden mithilfe der THz-Spektroskopie gemessen. Die THz-Spektren wurden zerlegt und die einzelnen Komponenten normalem Wasser, tetraedrisch angeordnetem Hydratwasser und ungeordneterem Hydratwasser zugeordnet. Das tetraedrisch angeordnete Wasser erzeugt eine Bande bei 195 cm^{-1} und ist am hydrophoben Teil des Alkohols lokalisiert. Die zweite Komponente zeigt eine Bande bei 165 cm^{-1} und wird dem Hydratwasser in der ersten Solvatationsschale zugeordnet. Die vermessenen, temperaturabhängigen Änderungen im THz-Spektrum von gelösten Alkoholketten können direkt mit Änderungen von Wärmekapazität, Entropie und freier Energie korreliert werden. Dabei ist überraschenderweise nicht das tetraedrisch angeordnete Wasser, sondern hauptsächlich das ungeordnete Hydratwasser für die temperaturabhängigen Änderungen von ΔC_p und ΔG verantwortlich. Der für den gelösten Stoff spezifische Unterschied in der freien Energie ist auf die Bildung von Kavitäten zurückzuführen und skaliert linear mit der Kettenlänge der Alkohole.

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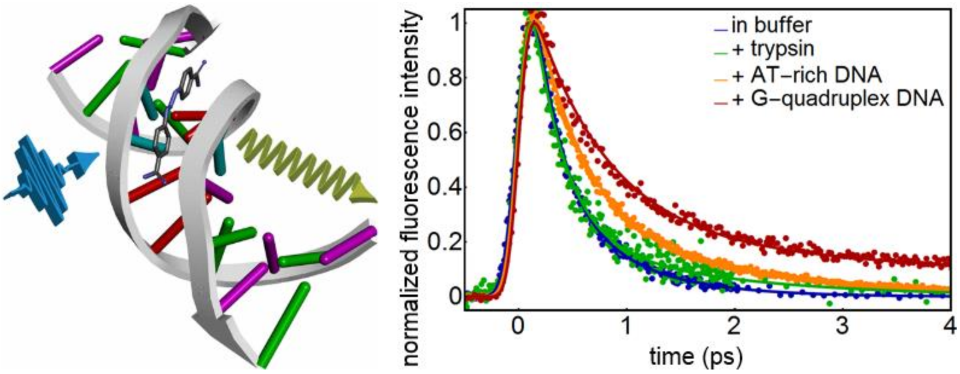
J. Phys. Chem. Lett., **2017**, 8, 1986 – 1992.

Ultrafast dynamics of a triazene: Excited-state pathways and the impact of binding to the minor groove of DNA and further biomolecular systems

Berenil is an aromatic diamidine with two amidinophenyl units linked by a triazene bridge. The molecule is the most widely used drug for treating sleeping sickness in animals and has many further pharmaceutical applications because of its high binding affinity to biomolecules like DNA or many enzymes. In the literature, berenil is often described as "non-fluorescent" both in the bound and unbound state. This points towards a short excited-state lifetime and ultrafast nonradiative deactivation channels on which the molecule's surrounding might have a significant impact. Femtosecond time-resolved fluorescence studies of berenil in various pure solvents, bound to trypsin, to the minor groove of AT-rich DNA, and to G-quadruplex DNA demonstrate that berenil in all cases exhibits a biexponential deactivation of the excited state within a few picoseconds after photoexcitation. Complementary ab-initio calculations disclose the origin of the biphasic excited-state motion which starts with the lengthening of the central N═N double bond, followed by a bicycle-pedal-type motion of the triazene bridge.



Left: Cartoon representation of berenil bound in the minor groove of AT-rich DNA where it is excited with a femtosecond pulse and subsequently fluoresces. Right: Transient fluorescence signal at an emission wavelength of 480 nm for berenil bound to different biomolecules.

Berenil ist ein aromatisches Diamidin mit zwei über eine Triazenbrücke verbundenen Amidinophenyleinheiten. Das Molekül ist das weitestverbreitete Medikament gegen die Schlafkrankheit bei Tieren und hat weitere zahlreiche pharmazeutische Anwendungen aufgrund der hohen Affinität, an Biomoleküle wie DNA oder so manche Enzyme zu binden. In der Literatur wird Berenil sowohl im ungebundenen als auch im gebundenen Zustand oft als „nicht fluoreszierend" beschrieben. Dies deutet auf eine sehr kurze Lebensdauer des angeregten Zustands und einen ultraschnellen, nichtstrahlenden Deaktivierungskanal hin, auf welchen die Umgebung des Moleküls einen signifikanten Einfluss haben könnte. Studien mit zeitaufgelöster Femtosekunden-Fluoreszenzspektroskopie an Berenil in unterschiedlichen Lösungsmitteln, gebunden an Trypsin, in der Minor Groove von AT-reicher DNA, oder an G-quadruplex DNA demonstrieren, dass Berenil in allen Fällen eine biexponentielle Deaktivierung des angeregten Zustands innerhalb weniger Pikosekunden nach der Anregung aufweist. Komplementäre ab-initio Berechnungen offenbaren den Ursprung dieses zweiphasigen Verhaltens im angeregten Zustand, welches mit einer Dehnung der zentralen N═N Bindung beginnt, gefolgt von einer Fahrradpedal-Bewegung der Triazenbrücke.

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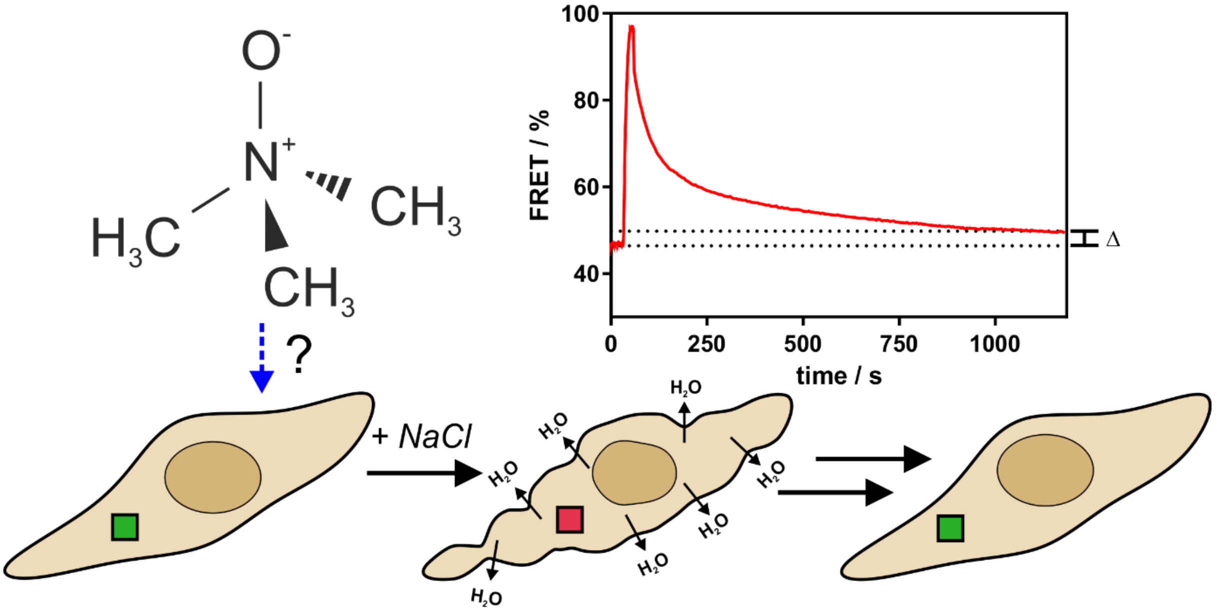
D. Gnutt, O. Brylski, E. Edengeiser, M. Havenith, S. Ebbinghaus, *Mol. BiolSyst.*, **2017**, 13(11) 2218-2221.

Cells are a complex and crowded environment. Intracellular crowding effects have been shown to affect biomolecular structure and behaviour. Changes of the extracellular milieu could affect the cellular crowding. To prevent detrimental effects, cells use adaptation mechanisms to react to such conditions. Using fluorescent crowding sensors, we show that the initial response to osmotic stress is fast but imperfect, while the slow response renders cells more tolerant to stress, particularly in the presence of osmolytes. Our approach allows to understand crowding changes after stress with high spatio-temporal resolution and sets the stage to characterize crowding in perturbed cellular systems.



Lebende Zellen sind ein komplexer und dicht gedrängter Ort. Intrazelluläres Crowding hat Einfluss auf die Struktur und das Verhalten von Biomolekülen. Änderungen des extrazellulären Milieus können das intrazelluläre Crowding beeinflussen. Um schädliche Effekte zu vermeiden, benutzen Zellen Adaptations-Mechanismen als Reaktion auf solche Bedingungen. Mit Hilfe von fluoreszenz-basierten Crowding Sensoren zeigen wir, dass die initiale Antwort auf osmotischen Stress zwar schnell, aber nicht perfekt ist. Die langsame Antwort erhöht die zelluläre Toleranz gegenüber Stress, insbesondere in Anwesenheit von Osmolyten. Unser Ansatz erlaubt das Verständnis von Crowding Änderungen mit hoher räumlicher und zeitlicher Auflösung und stellt die Grundlage dar zur weiteren Charakterisierung von Crowding-Änderungen nach zellulären Perturbationen.

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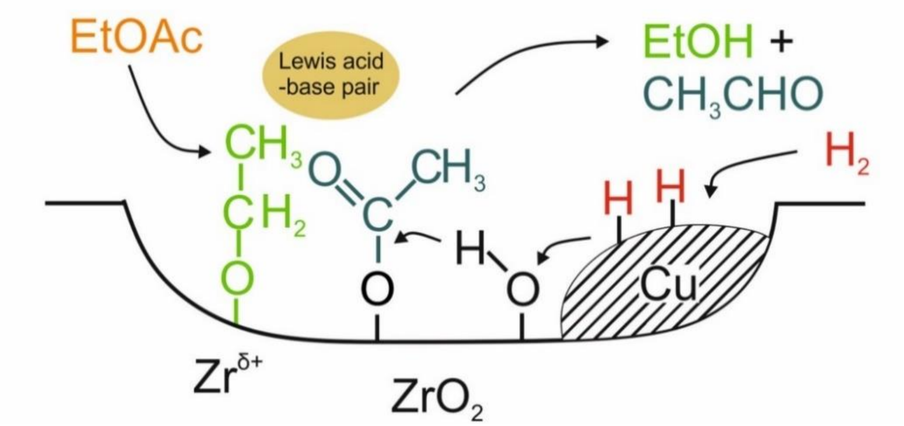
J. Schittkowski, K. Tölle, S. Anke, S. Stürmer, M. Muhler, *J. Catal.*, **2017**, 352, 120-129.

On the bifunctional nature of Cu/ZrO_2 catalysts applied in the hydrogenation of ethyl acetate

Cu/ZrO_2 catalysts with different Cu loadings were obtained by co-precipitation The catalytic hydrogenation of ethyl acetate to ethanol was studied as test reaction for metal-support interactions at ambient pressure in the temperature range from 463 K to 513 K. The hydrogenation was established as a reproducible probe reaction in the kinetic regime by determining optimal reaction parameters without deactivation or thermodynamic limitations. Power-law kinetics were determined yielding an apparent activation energy of 74 kJ mol^{-1} and reaction orders of 0.1 to 0.3 for H_2 and -0.4 to 0.1 for ethyl acetate in the temperature range from 473K to 503 K. Metallic Cu was found to be essential for the hydrogenation, but the catalytic activity was not proportional to the Cu surface area derived from N_2O decomposition and temperature-programmed H_2 desorption experiments identifying Cu/ZrO_2 as bifunctional catalyst. The acidic sites of the ZrO_2 matrix were probed by temperature-programmed experiments with ethyl acetate and NH_3. Cu^0 is assumed to provide atomic hydrogen by dissociative adsorption and spillover, but the reaction rate is more affected by the tight contact between the embedded Cu nanoparticles and the X-ray amorphous ZrO_2 matrix.



Es wurden Cu/ZrO_2-Trägerkatalysatoren mit verschiedenen Cu-Beladungen durch Kofällung hergestellt. Die Hydrierung von Ethlyacetat zu Ethanol wurde als Testreaktion für Metall-Träger-Wechselwirkungen bei atmosphärischem Druck im Bereich von 463 K bis 513 K eingesetzt. Durch die geeignete Wahl der Reaktionsbedingungen wurde gewährleistet, dass die Reaktion unter kinetisch kontrollierten Bedingungen ohne Limitierung durch Desaktivierung oder den thermodynamischen Gleichgewichtsumsatz erfolgte. Die Kinetik wurde durch einen Potenzansatz mit Reaktionsordnungen von 0.1 bis 0.3 für H_2 und -0.4 bis 0.1 für Ethlyacetat im Temperaturbereich von 473 K bis 503 K bestimmt. Metallisches Cu war für die Hydrierung essentiell, aber die katalytische Aktivität war nicht proportional der Cu-Oberfläche, die durch N_2O-Frontalchromatographie und temperaturprogrammierte H_2-Desorptionsexperimente (TPD) bestimmt wurde. Damit konnte Cu/ZrO_2 als bifunktionaler Katalysator identifiziert werden. Die sauren Zentren der ZrO_2-Matrix wurden durch TPD-Experimente mit Ethylacetat und NH_3 untersucht. Es wird davon ausgegangen, dass Cu^0 atomaren Wasserstoff durch dissoziative Adsorption und *Spill-over* bereitstellt. Die Reaktionsgeschwindigkeit ist jedoch mehr durch den engen Kontakt zwischen den eingebetteten Cu-Nanopartikeln und der röntgenamorphen ZrO_2-Matrix bestimmt.

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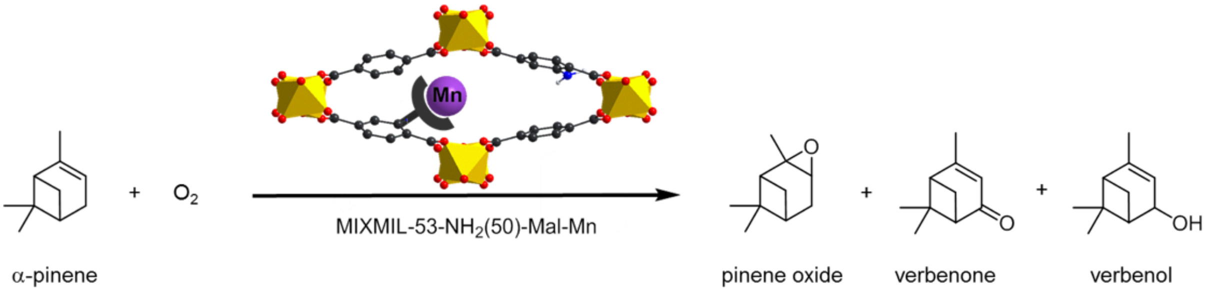
Yasmin S. Raupp, Ceylan Yildiz, Wolfgang Kleist, Michael A.R. Meier, *Appl. Catal. A - Gen.*, **2017**, 546, 1-6.

Aerobic oxidation of α-pinene catalyzed by homogeneous and MOF-based Mn catalysts

Within the present work, a mixed-linker metal-organic framework with MIL-53(Al) structure containing equal amounts of terephthalate and 2-aminoterephthalate linker molecules was successfully synthesized and further modified in a two-step post-synthetic modification (PSM) reaction to immobilize well-defined manganese complexes at the functional side groups of the organic linkers. Thorough characterization using a variety of different analytical and spectroscopic methods (XRD, NMR, IR, AAS, N_2 physisorption) confirmed the phase purity of the crystalline material and the successful immobilization of the Mn complexes in the pore structure. This resulted in a novel type of catalyst material for the liquid phase oxidation of α-pinene using molecular oxygen as oxidant and diethyl carbonate as a sustainable co-solvent. Screening of a variety of important reaction parameters revealed optimized reaction conditions and demonstrated that the MOF-based Mn catalyst exhibited a remarkable activity, which was comparable to that of homogeneously dissolved Mn salts. Furthermore, the solid catalyst could be easily separated and reused in five catalytic cycles without a significant loss of activity. A hot filtration test proved that the reaction proceeded mainly via a truly heterogeneous pathway, although minor contributions of dissolved Mn species could not be completely excluded.



Oxidation of α-pinene catalyzed by MOF-based catalyst MIXMIL-53-NH_2(50)-Mal-Mn.

Im Rahmen dieser Arbeit wurde eine Metall-organische Gerüstverbindung mit gemischten organischen Linkern hergestellt, die in einer zweistufigen postsynthetischen Modifizierungsreaktion (PSM) weiter umgesetzt wurde, um an den funktionellen Seitengruppen der organischen Linker definierte Mn-Komplexe zu immobilisieren. Mittels einer ausführlichen Charakterisierung mit unterschiedlichen analytischen und spektroskopischen Methoden (XRD, NMR, IR, AAS, N_2-Physisorption) konnten die Phasenreinheit des Produkts und die erfolgreiche Immobilisierung der Mn-Spezies in den Poren bestätigt werden. Das resultierende neuartige Katalysatormaterial wurde in der Flüssigphasenoxidation von α-Pinen eingesetzt, wobei molekularer Sauerstoff als Oxidationsmittel und Diethylcarbonat als nachhaltiger Lösungsmittelbestandteil zum Einsatz kamen. Durch Variation wichtiger Parameter konnten optimierte Reaktionsbedingungen ermittelt werden, unter denen der MOF-basierte Katalysator eine hohe Aktivität zeigte, die mit der gelöster, homogener Mn-Salze vergleichbar war. Der neue Heterogenkatalysator konnte erfolgreich abgetrennt und ohne nennenswerten Aktivitätsverlust in fünf aufeinanderfolgenden katalytischen Zyklen eingesetzt werden. Ein Filtrationstest bestätigte, dass die Reaktion überwiegend über einen heterogenen Reaktionsmechanismus verlief, obwohl eine Beteiligung gelöster Mn-Spezies in geringem Ausmaß nicht komplett ausgeschlossen werden konnte.

Theoretical Chemistry – Theoretische Chemie

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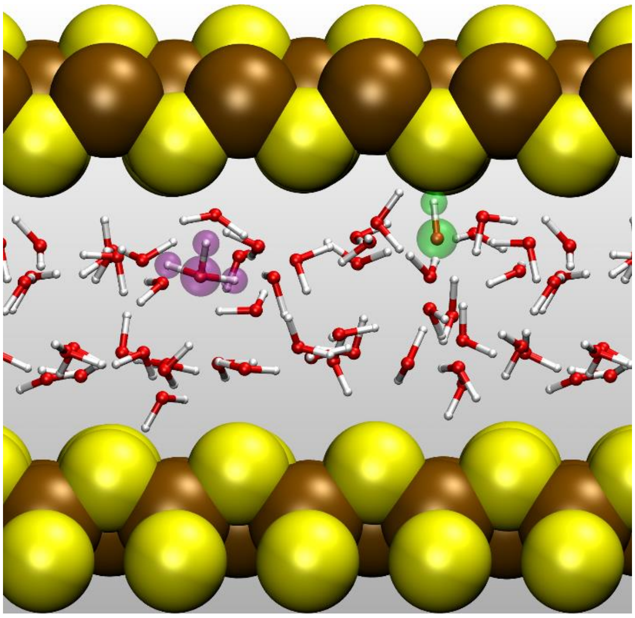
D. Munoz-Santiburcio, D. Marx,
Phys. Rev. Lett., **2017,** 119, 056002.

Nanoconfinement in Slit Pores Enhances Water Self-Dissociation

Using ab initio molecular dynamics simulations, we discovered that the pKa of pure water increases simply as a result of nanoconfinement of this liquid in between slit pores (see figure), thus resulting in enhanced self-dissociation. We have shown that this fundamental effect is not related to the altered polarity of water, but rather due to different polarization fluctuations in the nanoconfining environment in comparison to the homogeneous bulk phase.



Mit ab initio Simulationen haben wir entdeckt, dass der pKa Wert von reinem Wasser ausschließlich aufgrund seiner Beschränkung in einer Schlitzpore (siehe Abbildung) vergrößert wird, was mit einer erhöhten Selbstdissoziation einhergeht. Wir haben gezeigt, dass dieser grundlegende Effekt nichts mit der veränderten Polarität von Wasser zu tun hat, sondern stattdessen durch unterschiedliche Polarisations-fluktuationen in Schlitzporen relativ zur homogenen Volumenphase hervorgerufen wird.

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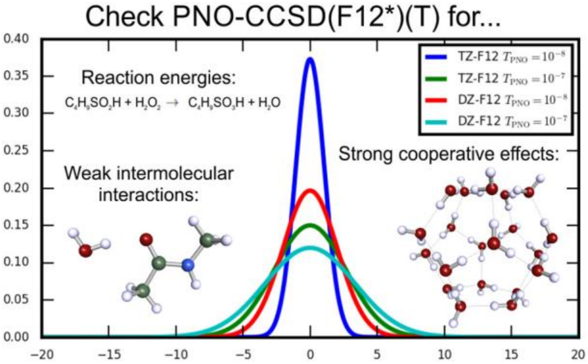
G. Schmitz, C Hättig, *J. Chem. Theory Comput.*, **2017**, 13, 2623-2633.

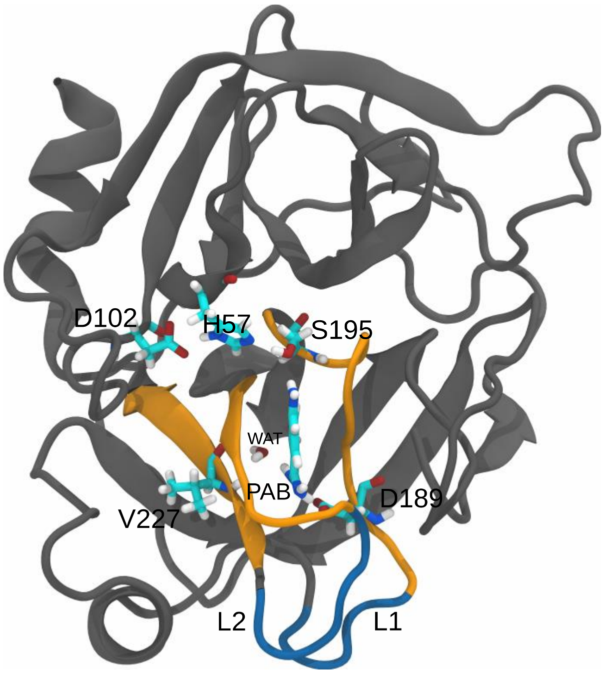
Accuracy of Explicitly Correlated Local PNO-CCSD(T).

New PNO-based local correlation methods that have been developed during the last years allow accurate Coupled Cluster calculations with reduced computational costs. In this work we took a deeper look at the explicitly correlated local PNO-CCSD(F12*)(T0) and PNO-CCSD(F12)(T) methods and assessed their accuracies using well-established benchmark sets for reaction energies and weak intermolecular interactions and a water cluster with strong cooperative many-body effects. For reaction energies a close agreement with the canonical methods is observed, and chemical accuracy can be reached. Also for weak intermolecular interactions the accuracy is easily controlled, and the methods even allow for improving existing benchmark data.



Distributions of the errors in kJ/mol for reaction and interaction energies computed with PNO-CCSD(F12)(T) in different basis sets and PNO selection thresholds .*

Neue PNO-basierte lokale Korrelationsmethoden, die in den letzten Jahren entwickelt wurden ermöglichen genaue Coupled-Cluster-Rechnungen zu reduzierten Rechenkosten. In dieser Arbeit haben wir die explizit-korrelierten lokalen PNO-CCSD(F12*)(T0)- und PNO-CCSD(F12*)(T)-Methoden genauer untersucht und ihre Genauigkeit anhand gut etablierter Testsätze für Reaktionsenergien und schwache intermolekulare Wechselwirkungen und einem Wasser-Cluster mit starken kooperativen Vielteilcheneffekten evaluiert. Für Reaktionsenergien wurde eine sehr gute Übereinstimmung mit den kanonischen Methoden beobachtet und die Methoden erreichen chemische Genauigkeit. Auch fuer schwache intermolekulare Wechselwirkungen erlauben diese Methoden eine gute Kontrolle der Genauigkeit und ermöglichen sogar die Verbesserung existierender Referenzdaten.



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S. M. Gopal, F. Klumpers, C. Herrmann, L. Schäfer. *Phys. Chem. Chem. Phys.*, **2017**, 19,10753-10766.

Solvation plays an important role in virtually all biomolecular recognition and binding processes. However, the consequences of changes in solvation conditions often remain elusive. In a collaboration of theoretical and physical chemists at RUB, we combined isothermal titration calorimetry (ITC) and molecular dynamics (MD) simulations to investigate the effect of solvent composition on the thermodynamics of protein–ligand binding. We studied the binding of *p*-aminobenzamidine (PAB) to trypsin in various water/methanol mixtures as a model system for a biomolecular complex.

Our ITC experiments show that the free energy of binding changes only very little with methanol concentration, and that this small change is due to strong enthalpy–entropy compensation. The MD and free energy simulations not only reproduce the experimental binding free energies, but also provide atomic-level insights into the mechanisms behind the thermodynamic observations. The more favorable binding enthalpy at increased methanol concentrations (compared to pure water) is attributed to stronger protein–ligand and intramolecular protein–protein interactions. The stronger protein–ligand interaction is linked to a small-scale conformational rearrangement of the L2 binding pocket loop, which senses the solvent environment. Remarkably, the stronger interactions do not substantially reduce the configurational entropy of the protein. Instead, the more disfavorable entropy contribution to the binding free energy at increased methanol concentrations is due to the desolvation of the ligand from the bulk, which is more favorable in pure aqueous solution than in water/methanol mixtures. Our work thus underpins the importance of including conformational flexibility, even for an overall rather rigid complex, because even small-amplitude motions can significantly alter the binding energetics. Furthermore, the ability of our combined ITC/MD approach to assign different thermodynamic contributions to distinct conformational states might contribute to an enhanced understanding of biomolecular binding processes in general.

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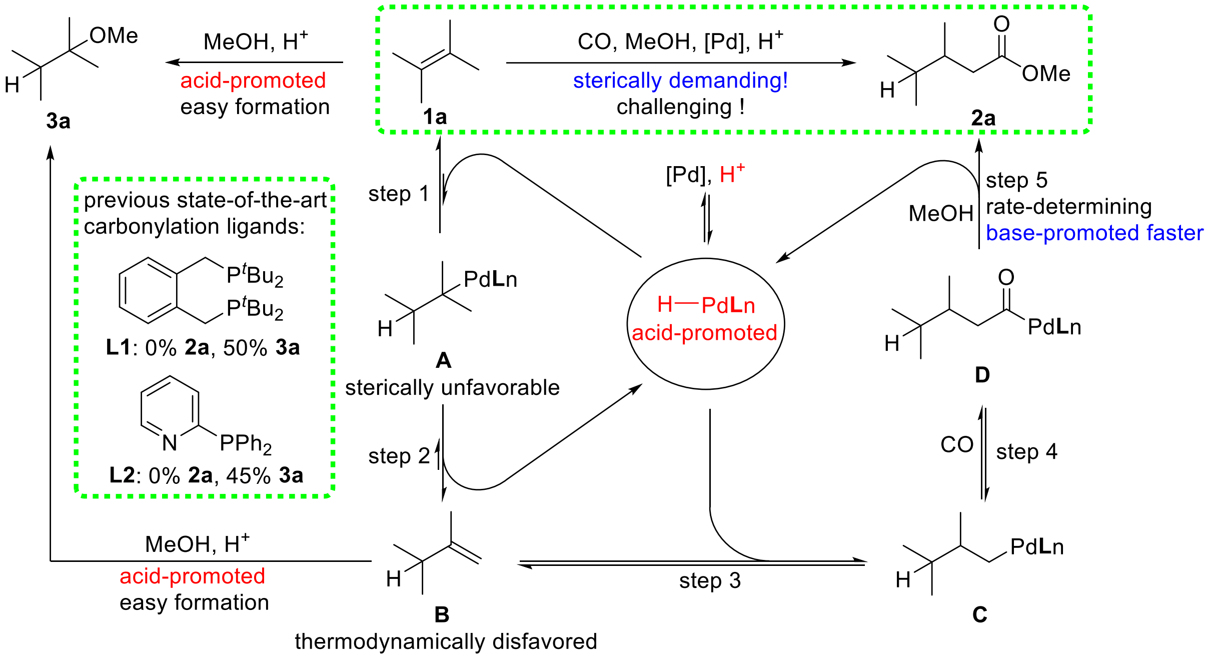
K. Dong, X. Fang, S. Gülak, R. Franke, A. Spannenberg, H. Neumann, R. Jackstell, M. Beller, *Nat. Commun.*, **2017**, 8, 14117

Highly active and efficient catalysts for alkoxycarbonylation of alkenes

Carbonylierungen von Alkenen gehören zu den wichtigsten industriellen Prozessen in der homogenen Katalyse. Trotz der großen Fortschritte, die auf diesem Gebiet gemacht wurden, bleibt die Verbesserung der Aktivität derartiger Katalysatorsysteme von großer Bedeutung, um das Anwendungsspektrum derartiger Reaktionen zu erweitern. Durch rationales Ligandendesign konnte ein neues auf Palladium basierendes Katalysatorsystem gefunden werden. Das System eignet sich, um eine große Vielfalt an Substraten umzusetzen und unter milden Bedingungen zu den entsprechenden Estern zu konvertieren. Es zeichnet sich insbesondere bei der Umsetzung industrieller Großchemikalien durch außerordentlich hohe Aktivität und Selektivität aus.



Carbonylation reactions of alkenes constitute the most important industrial processes in homogeneous catalysis. Despite the tremendous progress in this transformation, the development of advanced catalyst systems to improve their activity and widen the range of feedstocks continues to be essential for new practical applications. We therefore set out to rationally design and synthesize a novel palladium catalyst based on 1,2-bis((tert-butyl(pyridin-2-yl)phosphanyl)methyl)benzene L3 (pytbpx). Application of this system now allows, for the first time ever, a general alkoxycarbonylation of sterically hindered and demanding olefins. The usefulness of this catalyst is demonstrated by the conversion of all kinds of tetra-, tri-, and 1,1-disubstituted alkenes as well as natural products and pharmaceuticals into the desired esters in excellent yield under mild conditions. Industrially relevant bulk olefins including ethylene are functionalized with unpreceded activity (TON: >1,425,000; TOF: 44,000 h-1 for initial 18 h) and selectivity (>99%).

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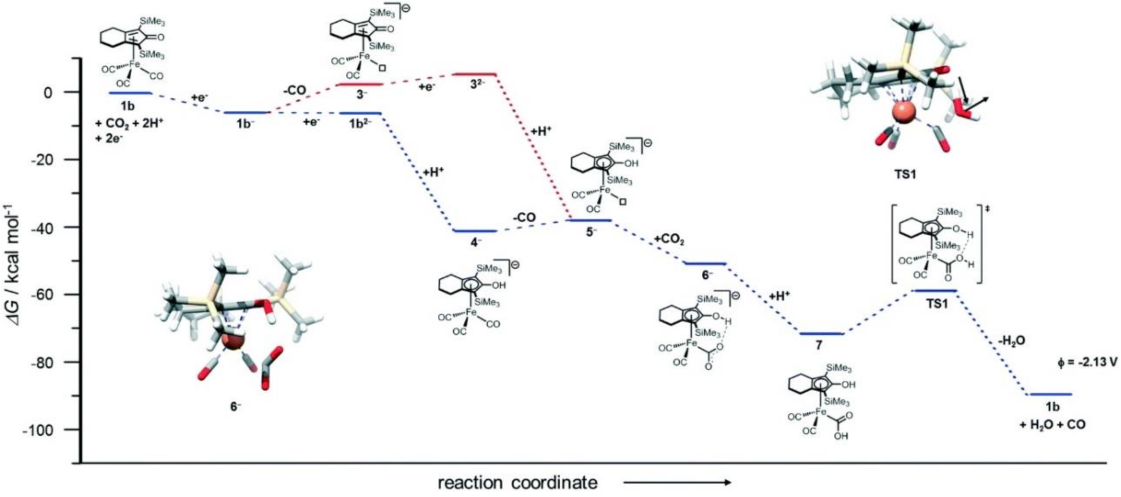
A.R. Hernández, H. Junge, M. Beller, M. Roemelt, R. Francke *Cat. Sci. Technol.* **2017**, 7, 459-465

Cyclopentadienone iron complexes as efficient and selective catalysts for the electroreduction of CO_2 to CO

Herein, we report the use of molecularly-defined cyclopentadienone iron(0) complexes as selective and efficient catalysts for the electrochemical conversion of CO_2 to CO in the absence of Brønsted acids. Quantum chemical calculations together with cyclic voltammetry allowed for a detailed insight into the probable mechanism of the observed reaction. It has been found that the initial release of CO and subsequent binding of CO_2 to the metal center in the required η^1-CO_2 fashion is only feasible after twofold reduction of the stable form of the catalyst. As the twofold reduced catalyst is highly basic it is able to abstract a proton from the solvent and/or the electrolyte. A second protonation following the CO_2 binding triggers a concerted sequence of intramolecular O-H bond formation and C-O bond breaking leading to the release of water. Importantly, the key to the remarkable behavior of the investigated complexes is the cooperative interaction between the cyclopentadienone ligand and the metal center. The local proton source formed on the ligand facilitates both, the binding of CO_2 to the metal center and the C-O bond cleavage.



Proposed reaction mechanism for selective electrochemical CO_2 reduction

Diese Arbeit handelt von der Benutzung von molekular definierten Cyclopentadienon-Eisen(0)-Komplexen als selektive und effiziente Katalysatoren für die elektrochemische Umwandlung von CO_2 zu CO in Abwesenheit von Brønsted Säuren. Quantenchemische Berechnungen zusammen mit cyclischer Voltammetrie erlauben detaillierte Einblicke in den wahrscheinlichen Reaktionsverlauf. Es konnte gezeigt werden, dass die anfängliche Abgabe von CO und die anschliessende Bindung von CO_2 an das Metallzentrum nur nach zweimaliger Reduktion des Katalysators wahrscheinlich sind. Da der reduzierte Katalysator stark basisch ist, ist er in der Folge dazu in der Lage ein Proton vom Solvens oder dem Leitsalz zu abstrahieren. Eine anschliessende zweite Protonierung löst eine konzertierte Abfolge einer intramolekularen O-H Bindungsknüpfung und eines C-O Bindungsbruch aus, welche zur Abspaltung von Wasser führt. Die aussergewöhnliche beobachtete Reaktiviät wird nur durch die kooperative Wechselwirkung zwischen dem Cyclopentadienon-Liganden und dem Metallzentrum ermöglicht. Die auf dem Liganden lokal gebildete Protonenquelle erleichtert sowohl die Bindung von CO_2 an das Metallzentrum als auch den C-O Bindungsbruch.

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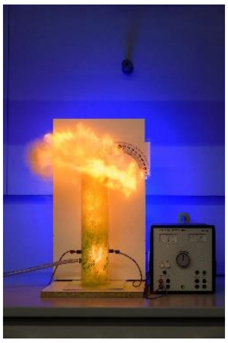
K. Sommer, C. Toschka, L. Schröder, T. P. Schröder, H. Steff, R. A. Fischer, *CHEMKON* **2017**, 24, 13-19.

Model experiments for chemistry education
A contribution to the definition of the term model experiment and the determination of the modeling degree

What are model experiments? Model experiments play an important role in chemistry education. They are always used in the chemical context, if experiments showing the original situation are unavailable due to their complexity, accessibility, risk potential, handling and/or costs. However, the term is only vaguely defined in didactic journals and schoolbooks. Yet, the definition of the term model experiment is important for both science research and teaching to evaluate and improve existing model experiments. This article defines the term model experiment for chemistry education for the first time. This definition will allow discrimination from simulation models, theoretical models and functional models.

Based on this definition, the different characteristics of model experiments can also be determined quantitatively for experiments. We call this the modelling degree. It allows more precise statements about the proximity and relationship between model and original.



Mit der Low-Cost-Hartmannapparatur eine Staubexplosion modellieren

Was sind Modellexperimente? Modellexperimente spielen im Chemieunterricht eine wichtige Rolle. Sie werden immer dann eingesetzt, wenn Experimente, die originale Sachverhalte widerspiegeln, aus Gründen der Komplexität, der Zugänglichkeit, des Gefahrenpotentials, der Handhabung und/oder der Kosten nicht zugänglich sind. In der chemiedidaktischen Literatur sowie in Chemie-Schulbüchern besteht jedoch eine große Unschärfe bei dem Gebrauch dieses Begriffes. Für die Auseinandersetzung mit diesem Themenfeld ist es sowohl für die chemiedidaktische Forschung als auch für den Chemieunterricht wichtig, den Begriff Modellexperiment zu definieren, um u. a. bestehende Modellexperimente kritisch zu prüfen. Im vorliegenden Beitrag wird der Begriff Modellexperiment erstmalig für den Chemieunterricht Kriterien geleitet definiert. Diese Definition soll eine bewusste Abgrenzung der Modellexperimente von Simulationsmodellen, Denkmodellen und Funktionsmodellen etc. ermöglichen. Darauf aufbauend kann sich bei Experimenten, welche diese Kriterien eines Modellexperimentes aufweisen, die Quantität der modellierten Merkmale unterscheiden. Das wird im Modellierungsgrad ausgedrückt. Er erlaubt präzisere Aussagen über die Beziehung zwischen Modell und Original.

EPR-Spectroscopy

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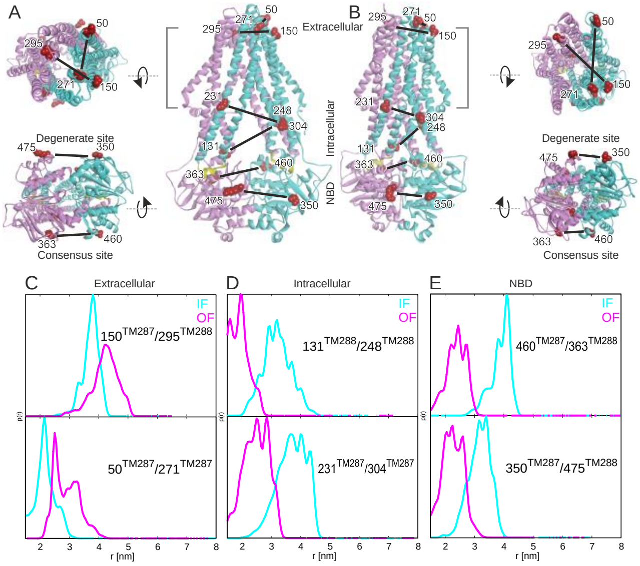
M.H. Timachi, C.A. Hutter, M. Hohl, T. Assafa, S. Boehm, A. Mittal, M.A. Seeger, E. Bordignon, *eLife*, **2017**, 6, E20236

Exploring conformational equilibria of a heterodimeric ABC transporter

ATP binding cassette (ABC) exporters are found in all phyla of life and play a key role in the transport of a variety of molecules across cell membranes using the energy of ATP hydrolysis. Around half of the forty human ABC exporters have two functionally non-equivalent ATP binding sites, which includes transporters of major clinical importance such as the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR).
Here we present a comprehensive site-directed spin labelling EPR study supported by biochemical assays on a bacterial ABC heterodimeric transporter to understand at the molecular level how ABC exporters perform their function.



Two states of an ABC transporters with EPR spin probes attached, and simulated interspin distance distributions.

ABC-Transporter bilden eine große Familie von Membranproteinen, die als gemeinsames Strukturelement eine ATP-bindende Kassette (ABC) besitzen und spezifische Substrate aktiv über eine Zellmembran transportieren durch die Bindung und Hydrolyse von ATP. Rund die Hälfte der vierzig menschlichen ABC-Transporter hat zwei funktionell nichtgleichwertige ATP verbindliche Seiten, einschließlich der klinischen Hauptwichtigkeit wie die Zystische Fibrose Transmembrane Leitfähigkeitsregler (CFTR).
Hier präsentieren wir eine umfassende EPR Studium auf einem bakteriellen ABC Transporter, um am molekularen Niveau zu verstehen, wie ABC-Transporter ihre Funktion durchführen.

List of Publications 2017

Analytical Chemistry

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EPR-Spectroscopy

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Awarded PhD in 2017

Name	given Name	Supervisor	Topic	Date
Ferreira Beltrán	Madeline	Prof. Dr. M. Hollmann	Funktionelle Charakterisierung von Spleißvarianten der GluN3B-Untereinheit	03.03.2017
Tseng	Jo-Chi	PD Dr. C. Weidenthaler	Microstructure Analysis of Nanosized Materials Based on X-Ray Diffraction Study: A Practical Protocol	06.03.2017
Maaske	André Juan	Prof. Dr. M. Tenbusch	Treatment of allergic asthma by gene based immunizations that induce specific targeting of antigens toward dendritic cells	09.03.2017
Ganassin	Alberto	Prof. Dr. W. Schuhmann	Intrinsic Catalytic Properties of Electrocatalysts, a Model Surface Approach	10.03.2017
Lapuente	Dennis	Prof. Dr. M. Tenbusch	Evaluation of IL-1β and IL-18 as genetic adjuvants in adenoviral immunizations against influenza A viruses	10.03.2017
Pereira Lemos	Sandra da Conceição	Prof. Dr. M. Hollmann	Regulation of AMPA receptors by type II-TARPs	13.03.2017
Schittkowski	Julian	Prof. Dr. M. Muhler	Kinetic and calorimetric studies of structure-activity correlations in copper-based hydrogenation catalysts	20.03.2017
Cheng	Hsiu-Wei	Prof. Dr. M. Stratmann	Probing the Solid/Liquid Interfacial Structure of Ionic Liquids and Battery Fluids by Surface Force Measurements: Influence of water, ions and surface chemistry in interfacial structuring	31.03.2017
Eckert	Rene	Prof. Dr. F. Schüth	Mechanokatalytische CO-PROX	31.03.2017
Mendes Burak	Jorge Augusto	Dr. R. Rinaldi	Raney Ni stability and characterization upon different systems and solvents	31.03.2017
Nese	Valentina	Prof. Dr. F. Schüth	Solid Catalysts for the Production of 5-Hydroxymethylfurfural and 2,5-Furandicarboxylic acid	31.03.2017
Siegmund	Daniel	Prof. Dr. N. Metzler-Nolte	Rhenium(I) N-Heterocyclic Carbene Complexes as Novel Organometallic Antibacterial Agents	07.04.2017
Höcker	Peer Henning	Prof. Dr. M. Hollmann	Identifizierung für die AMPA-Rezeptormodulation relevanter Domänen von stargazin	21.04.2017
Sharma	Abhishek	Prof. Dr. J. S. McCaskill	Microscale Transport of Informational Molecules in Smart Electronic Devices	25.04.2017
Kaufmann	Matin Alexander	Prof. Dr. M. Havenith-Newen	Infrarotspektroskopie von Glycin, Glycin-Wasser-Aggregaten und Tropyl isoliert in Heliumtröpfchen	28.04.2017

Kim	Jiyeon	Prof. Dr. R. A. Fischer	Organometallic Chemistry of Transition Metal-Group 13 Complexes and Metal-Organic Precursor Synthesis for ALD Cobalt Oxide Thin Films	28.04.2017
Kondati Natarajan	Suresh	Prof. Dr. J. Behler	Computer Simulations of Copper-Water Interface	05.05.2017
Leicht	Daniel	Prof. Dr. M. Havenith-Newen	Helium Nanodroplet Isolation Infrared Spectroscopy of Organic Radicals and their Complexes with Small Molecules	05.05.2017
Mittal	Sumit	Prof. Dr. E. Sánchez-García	Small Molecule Modulation of Protein-Protein Interactions: A Computational Study	05.05.2017
Klewe	Kristoffer	Prof. Dr. J. Rassow	Insertion und Oligomerisierung des trypanolytischen Faktors Apolipoprotein L1 (ApoL1) in mitochondrialen Membranen	12.05.2017
Schröder	Thomas Philipp	Prof. Dr. K. Sommer	Validierungsparameter für Schulexperimente - Dargestellt an Modellexperimenten für Industrielle Prüfverfahren	15.05.2017
Klumpers	Fabian	Prof. Dr. Ch. Herrmann	Biophysikalische Charakterisierung des Faltungsmechanismus der Nore1A SARAH Domäne und des Einflusses des Solvens auf die Bindung von p-Aminobenzamidin an Trypsin	30.06.2017
Kadam	Pritam Eknath	Prof. Dr. W. Sander	Matrix Isolation of Highly Reactive Organic Intermediates	07.07.2017
Mieres Pérez	Joel	Prof. Dr. W. Sander	High-Spin Nitrenes: A Matrix Isolation Study	07.07.2017
Böing	Marion	Prof. Dr. B. Brand-Saberi	Charakterisierung des Transkriptionsfaktors Math6 als essentieller Regulator der Plazentaentwicklung	07.07.2017
Kutsch	Miriam	Prof. Dr. Ch. Herrmann	Molecular mechanisms of human guanylate binding protein complexes	07.07.2017
Strippel	Christian Georg	Prof. Dr. K. Sommer	Naturwissenschaftliche Erkenntnisgewinnung an chemischen Inhalten vermitteln - Konzeption und empirische Untersuchung einer Ausstellung mit Experimentierstation	20.07.2017
Heß	Rebecca Carine Julia	Prof. Dr. med. K. Überla	Beeinflussung der antiviralen Antikörperproduktion durch differentielle Stimulation der angeborenen Immunantwort mit viralen Oberflächenproteinen	28.07.2017
Martínez Fagundo	Danae	Prof. Dr. F. Schulz	Approaches towards chemoselective conjugation of Polyketide Synthases and $in vivo$ localization within $Saccharopolyspora erythraea$ filaments	15.08.2017

Kracht	Octavia Natascha	Prof. Dr. R. Kourist	Biokatalytische Diversität der Terpenbildung in Pflanzen und Bakterien	19.09.2017
Altin	Abdulrahman	Prof. Dr. A. Erbe	Cyclodextrin for Zinc Corrosion Protection	22.09.2017
Seidel	Sebastian	Prof. Dr. M. Havenith-Newen	Single-Conformation Spectroscopy of Biomolecular Building Blocks and their Microsolvated Clusters in a Molecular Beam	22.09.2017
Hante, geb. Schwedler	Inke	Prof. Dr. R. A. Fischer	Functional Metal-Organic Frameworks Targeted Design and Modification of Advanced Properties of MOFs via Organic Linker Functionalisation	22.09.2017
Schürmann	Sonja Kristina	Prof. Dr. W. Grünert	Sulfidkatalyse ohne Koordinationslücken: Aktive Zentren auf Molybdänsulfid	27.09.2017
Duyckaerts	Nicolas	Prof. Dr. F. Schüth	$In-situ$ Hydrocracking of Fischer-Tropsch Hydrocarbons: How α-Olefins Influence the Final Product Distribution	29.09.2017
Feichtner	Kai-Stephan	Prof. Dr. V. Däschlein-Geßner	Methandiid-basierte Carbenkomplexe in Bindungsaktivierungsreaktionen	29.09.2017
Alsheikh Oughli	Alaa	Prof. Dr. W. Lubitz	Protective Matrices for Hydrogenases and Bio-inspired Catalysts	04.10.2017
Cwik	Stefan	Prof. Dr. A. Devi	Metal nitride and metal disulfide thin films via CVD: Exploring the diversity of all nitrogen coordinated rare earth and group 6 precursors	04.10.2017
Rodríguez Maciá	Patricia del Rosario	Prof. Dr. W. Lubitz	From Hydrogenases to Molecular Catalysts: Electrochemical and Spectroscopic Investigations	04.10.2017
Barwe	Stefan	Prof. Dr. W. Schuhmann	The two Janus faces in oxygen electrocatalysis: Activity versus stability of transition metal based electrocatalysts	05.10.2017
Eßmann	Vera	Prof. Dr. W. Schuhmann	Analytical applications of bipolar electrochemistry - From open to closed to localised systems	05.10.2017
Dodekatos	Georgios	Dr. Harun Tüysüz	Copper-Cobalt-Based Catalysts and Gold/Titania Nanostructures for Thermocatalytic and Surface Plasmon-Assisted Glycerol Oxidation	06.10.2017
Xiong	Yan	Dr. F. Marlow	Nano-Sized BaTiO~3 and TiO2 in Photochemical Energy Conversion Systems	06.10.2017
Stapf	Stefanie	Prof. Dr. N. Plumeré	Viologen Polymers for Reversible Hydrogen Oxidation and Hydrogen Generation in Redox Hydrogels	06.10.2017

Cruz Zaragoza	Luis Daniel	Prof. Dr. R. Erdmann	New insights into *de novo* synthesis of peroxisomes and into alternative peroxisomal protein import pathways in *Saccharomyces cerevisiae*	09.10.2017
Efing	Nicolas	Prof. Dr. K. Sommer	Gespräche über ein Low Cost Aräometer Entwicklung und Pilotierung eines methodischen Vorgehens zur effizienten Untersuchung von Eltern-Kind-Interaktion im Lehr-Lern-Arrangeme	09.10.2017
Bäumer	Alexander	Prof. Dr. M. Havenith-Newen	Terahertz-Spektroskopie solvatisierter Biomoleküle	13.10.2017
Senske	Michael	Prof. Dr. M. Havenith-Newen	Protein Stability in Crowding and Confinement	13.10.2017
Breitkreuz	Martin Jan	Prof. Dr. W. A. Linke	Charakterisierung des Redoxzustandes von Titin und Bedeutung der Titinoxidation für die Eigenschaften entfalteter Titindomänen	20.10.2017
Knossalla	Johannes	Prof. Dr. F. Schüth	Utilizing Confined Space to Attain High Performance Catalysts and Support Materials	23.10.2017
Kuhn	Alexander Burkard	Prof. Dr. A. Schäfer	Untersuchungen zum Molekularen Mechanismus der Selbstassoziation Monoklonaler Antikörper	17.11.2017
Song	Huiqing	Prof. Dr. M. Muhler	ZnO/Cr_2O_3-based catalysts applied in methanol and higher alcohol synthesis	17.11.2017
Wütscher	Annika	Prof. Dr. M. Muhler	Der Einfluss von heterogenen Katalysatoren auf die Pyrolyse und den Abbrand von Kohlenstoffmaterialien	17.11.2017
Erdmann	Constanze	Prof. Dr. Ch. Herrmann	Charakterisierung von HCM und DCM auslösenden Mutationen in humanem kardialem α-Aktin	24.11.2017
Lopez	Francesca	Prof. Dr. W. Schuhmann	Enzyme electrodes based on polymer multilayer systems and nano-structured electrode surfaces for the development of novel biodevices	30.11.2017
Geiger	Simon	Prof. Dr. K. Mayrhofer	Stability investigations of iridium-based catalysts towards acidic water splitting	01.12.2017
Karle	Sarah	Prof. Dr. A. Devi	From Molecules to Materials: Rational Design and Development of Group 11 and Group 14 Complexes and Their Evaluation as Precursors for the Deposition of Metal and Metal Oxide Thin Films	01.12.2017
Murat	Yesim	Prof. Dr. M. Muhler	Synthese, Charakterisierung und Anwendung binärer $Ce_xZr_{1-x}O_2$-Mischmetalloxide	01.12.2017

Petuker	Anette	Dr. U.P. Apfel	Activation of Small Molecules with Iron and Nickel Complexes Comprising Tripodal Phosphines	06.12.2017
Balzerowski	Patrick	Prof. Dr. M. Havenith-Newen	Development of Spectrometers and Optical Components for the THz-Spectral Range and Nonlinear Experiments on Aqueous Solutions	08.12.2017
Gebhard	Maximilian	Prof. Dr. A. Devi	Plasma-Enhanced Atomic Layer Deposition of binary metal oxides as gas barrier layers on polmers	08.12.2017
Kayran	Yasin Uğur	Prof. Dr. W. Schuhmann	Fabrication and Characterization of Tunable Plasmonic Nanovoid Structures and Their Application in DANN/RNA Hybridization Assays	08.12.2017
Alsaoub	Sabine	Prof. Dr. W. Schuhmann	Synthesis of Stable Os-Complex Modified Polymers for the Applications in Biosensors, Biofuel Cells and Biosupercapacitors	08.12.2017
Klinkhammer	Christina	Prof. Dr. M. Havenith-Newen	Vibrationsspektroskopie von wässrigen Ytterbiumhalid-Lösungen und Plasma-behandeltem Glutathion	08.12.2017
Radhakrishnan	Soumya	Prof. Dr. W. Sander	Matrix Isolation and Solvation Studies of Reactive Intermediates	08.12.2017
Esser	Alexander	Prof. Dr. D. Marx	Theoretical THz Spectroscopy of Small Molecules in Water	11.12.2017
O'Donoghue	Richard	Prof. Dr. A. Devi	Atomic layer deposition of ZnO and Ga_2O_3 thin films as transparent semiconducting oxides: Influence of precursors on the film growth and characteristics	14.12.2017
Bertram	Cord	Prof. Dr. K. Morgenstern	Reaktionen durch heiße und solvatisierte Elektronen bei kryogenen Temperaturen	15.12.2017
Gonsberg	Anika	Prof. Dr. J. Tatzelt	Der Einfluss der Sekundärstruktur sekretorischer Proteine auf Sec61/Y-mediierten Proteintransport	15.12.2017
Quaranta	Vanessa	Dr. J. Behler	Neural Network Molecular Dynamics Studies of Water-Zinc Oxide Interfaces	15.12.2017
Dierks	Michael	Prof. Dr. F. Schüth	Hydrophobic Ni~2P/SiO~2 catalysts with improved stability for bio-oil hydrodeoxygenation	18.12.2017
Engelhardt	Jan	Prof. Dr. F. Schüth	Nanostructured Catalysts for Biomass Conversion	18.12.2017
Hugenbruch	Stefan Jürgen	Prof. Dr. S. DeBeer	X-ray spectroscopic and Mößbauer spectroscopic investigations of bioinorganic compounds and metalloenzymes	21.12.2017

Palmieri	Elena	Prof. Dr. G. Kiedrowski	Autocatalytic desymmetrization of prochiral compounds - Strategies to dictate and control self-replication in peptidic dynamic combinatorial libraries	22.12.2017