Einleitung/Preface

Wie jedes Jahr soll auch dieser Jahresbericht wieder einen kurzen Eindruck über die Vielfältigkeit der Forschung in der Fakultät für Chemie und Biochemie der Ruhr-Universität Bochum vermitteln. Wenn Sie zu den einzelnen Themen weitere Informationen wünschen, können Sie unter den angegebenen Adressen der Homepages der Arbeitsgruppen oder über die Homepage der Fakultät (http://www.chemie.rub.de/) vertiefte Einblicke erhalten.

Again this yearly report of the faculty of chemistry and biochemistry of the Ruhr-Universität Bochum is supposed to provide a flavor about the diversity of the research topics. If you need additional information to individual research topics, you are welcome to contact the research groups directly following the links, email addresses or telephone numbers provided with the research highlights. Moreover, you may find additional information on the website of the faculty (http://www.chemie.rub.de/).

Auch 2011 und insbesondere auch zu Beginn des Jahres 2012 hat sich wie immer sehr viel getan in der Fakultät, so dass ich sie nur mit einigen Links zu der entsprechenden Information leiten möchte:

As a matter of fact, many important things happened during the last year. I just want to guide you to some of the related information through the list of the following links:

- [http://www.ruhr-uni-bochum.de/solvation/](http://www.ruhr-uni-bochum.de/solvation/)
- [http://www.ruhr-uni-bochum.de/zemos/](http://www.ruhr-uni-bochum.de/zemos/)
- [http://www.rd.ruhr-uni-bochum.de/ifsc/](http://www.rd.ruhr-uni-bochum.de/ifsc/)
- [http://www.sfb558.de/](http://www.sfb558.de/)
- [http://www.ruhr-uni-bochum.de/ces/](http://www.ruhr-uni-bochum.de/ces/)
- [http://www.ruhr-uni-bochum.de/acc/terahertz/](http://www.ruhr-uni-bochum.de/acc/terahertz/)
- [http://www.chemie.ruhr-uni-bochum.de/gscb/](http://www.chemie.ruhr-uni-bochum.de/gscb/)

Bochum, October 2012

(Prof. Dr. Wolfgang Schuhmann)
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Peptide Nucleic Acids (PNAs) are non-natural DNA/RNA analogues with favourable physico-chemical properties and promising applications. Discovered nearly 20 years ago, PNAs have recently re-gained quite a lot of attention. In this Perspective article, advances on the preparation and utilisation of PNA monomers and oligomers containing metal complexes are summarized for the first time. These metal-conjugates have found applications in various research fields such as in the sequence-specific detection of nucleic acids, in the hydrolysis of nucleic acids and peptides, as radioactive probes or as modulators of PNA•DNA hybrid stability, and last but not least as probes for molecular and cell biology. The first author, Gilles Gasser was supported by a fellowship from the Alexander-von-Humboldt Foundation and is now Professor at the University of Zurich.

Energy efficient lighting is the need of the hour as nearly nineteen percent of global electricity generation is consumed for lighting – which is more than produced by hydro or nuclear stations and about the same that is produced from natural gas. Incandescent lamps, which are so far widely used, suffer from a poor luminous efficiency as most of the energy is converted to heat, and are replaced more and more by environmentally benign light sources such as light emitting diodes (LEDs) and compact fluorescent lamps (CFLs). Especially CFLs are extensively used as they consume less energy and have a longer rated life. But like all fluorescent lamps, CFLs also contain mercury which complicates their disposal and adds substantial health risks and environmental issues during manufacturing. A possible alternative in which Hg is replaced by an environmentally safe noble gas like Xe, has several advantages like immediate start, essential for special applications like lamps in facsimile, copying machines and car brake lights. However, the discharge efficiency of Xe is less compared to Hg. In addition, conversion of the yet shorter wavelength radiation to visible light results in an even larger energy loss compared to Hg based CFLs. In order to make Xe based CFLs competitive, a quantum yield of the used phosphor larger than 100% needs to be achieved. An ionic liquid (IL) assisted solvothermal method was developed that allowed to manufacture single phase, oxygen free, hexagonal NaGdF$_4$:Eu$^{3+}$ nanorods with a visible quantum efficiency of 187%.

Die Lanthanoide Ytterbium, Neodym, Praseodym und Erbium zeigen Photolumineszenz im Spektralbereich von ca. 800-1700 nm und sind aufgrund dieser Eigenschaft von einigem Interesse für eine Vielzahl von technologischen Anwendungen, z.B. für die optische Telekommunikation oder das Lumineszenz-Imaging im biomedizinischen Bereich. Die Lumineszenzefﬁzienz ist jedoch häufig gering, v.a. durch das Vorhandensein von multiphonon-induzierten Deaktivierungsmechanismen. Dabei spielen hochfrequente Ozillatoren wie z.B. C-H eine dominierende Rolle. Deren negative Auswirkungen können durch den Er- satz von C-H durch C-D-Einheiten stark abgeschwächt werden, was sich in der Regel deutlich positiv auf die Emissionsintensität auswirkt. Die neu entwickelten Lanthanoid-Cryptate \([\text{D30]}-\text{Ln-2}\) mit den Lanthanoiden Yb, Nd, Er und Pr (siehe Abbildung) können sehr leicht in perdeuterierter Form hergestellt werden und zeigen außerordentlich intensive Lumineszenz. Der Ytterbium-Cryptat \([\text{D30]}-\text{Yb-2}\) ist besonders effizient und besitzt enorm lange Lumineszenz-Abklingzeiten bis zu \(\tau = 91\ \mu\text{s}\). Damit ist er in etwa doppelt so effektiv wie die meisten bisher bekannten Ytterbium-Luminophore. Zudem zeigen diese Cryptate außergewöhnlich hohe Komplexstabilitäten in Lösung.

The lanthanoids ytterbium, neodymium, praseodymium, and erbium luminesce in the spectral range of ca. 800-1700 nm. This property makes them of considerable interest for a variety of technological applications, e.g. for optical telecommunication or for biomedical luminescence imaging. The luminescence efﬁciency, however, is often low, especially due to the presence of multiphonon-induced deactivation mechanisms, where high-frequency oscillators like C-H play a dominant role. Their negative influence can be mitigated by substitution of C-H for C-D units, which usually has a very positive effect on the emission intensity. The newly developed lanthanoid cryptates \([\text{D30]}-\text{Ln-2}\) with the lanthanoids Yb, Nd, Er, and Pr (siehe figure) can be synthesized easily in perdeuterated form and show extraordinarily intense luminescence. The ytterbium cryptate \([\text{D30]}-\text{Yb-2}\) is especially efficient and possesses enormously long luminescence lifetimes of up to \(\tau = 91\ \mu\text{s}\). It is approximately twice as efﬁcient as most of the previously known ytterbium luminophores. In addition, these cryptates show extraordinarily high complex stabilities in solution.
Metal-Organic Frameworks (MOFs) represent a modular and highly tunable class of hybrid materials exhibiting extraordinary porosity. The \([\text{M}_2\text{L}_2\text{P}]_n\) (M = Co, Ni, Cu, Zn; L = linear dicarboxylate linker; P = neutral pillar) MOF family has been extensively studied in recent years. All known \([\text{M}_2\text{L}_2\text{P}]_n\) derivatives exhibit either a tetragonal or a Kagome-type topology. We have successfully synthesized a novel derivative of the composition \([\text{Zn}_2(\text{BME-bdc})_2(\text{bipy})]_n\) (BME-bdc = 2,5-bis(2-methoxyethoxy)-1,4-benzenedicarboxylate; bipy = 4,4'-bipyridine) which crystallizes in an unexpected honeycomb-like topology with one-dimensional cylindrical channels. The key for the construction of the honeycomb-like topology is the disubstitution of the dicarboxylate linker, which has a major impact on the conformational freedom of the carboxylate groups. The flexible 2-methoxyethoxy groups of the BME-bdc linker act as “molecular gates” for incoming guest molecules, yielding in exceptionally high sorption selectivity for \(\text{CO}_2\) over \(\text{N}_2\) or \(\text{CH}_4\) both give rise to a polycrystalline, polar surface, which enhance the adsorptive properties. Our results underline the huge potential of targeted linker modification for the development of highly efficient adsorbents for gas separation and sensing.


A series of malonate complexes of dysprosium were synthesized. The steric bulkiness of the dialkylmalonato ligand employed was systematically varied and its influence on the resulting structural and physico-chemical properties that is relevant for metalorganic chemical vapor deposition (MOCVD) was studied. X-ray diffraction analysis revealed that the homoleptic *tris*-malonato Dy complexes are dimers with distorted square-face bicapped trigonal-prismatic geometry and a coordination number of eight. In an attempt to decrease the nuclearity and increase the solubility of the complexes in various solvents, the focus was to react these dimeric complexes with Lewis bases such as 2,2′-bipyridyl and pyridine. This resulted in monomeric *tris*-malonato *mono* Lewis base adduct complexes with improved thermal properties. Finally the silylmalonate adduct complex [Dy(dsml)3bipy] was successfully employed as a single source precursor (SSP) for growing DySi$_x$O$_y$ thin films by liquid injection MOCVD process.
Porous coordination polymers, like the copper dimer based HKUST-1, are novel functional materials with potential in gas storage and separation, sensing and catalysis. However, often a number of supramolecular isomeric structures are possible in principle, whereas experimentally only a single crystal phase can be synthesized. Using our recently developed first-principles derived force field for such systems, which accurately computes energies for network deformations, we have for the first time predicted the relative stability of possible isomeric structures for a metal-organic framework. We found HKUST-1 to prefer the tbo network topology, as it is observed experimentally, and could explain why this is the case. Furthermore, with an enlarged organic linker, the situation is reversed and the pto structure is formed, as it is found synthetically for the so called MOF-14. Our method is a first step towards the theoretical structure prediction of such hybrid materials.
The development of photoelectrodes for splitting water into hydrogen and oxygen is one of the major challenges in chemical solar energy conversion. We investigated photoelectrodes based on TiO$_2$-polyheptazine hybrid materials. Since both TiO$_2$ and polyheptazine are extremely chemically stable, these materials are highly promising candidates for fabrication of photoanodes for water photooxidation. We provided for the first time clear experimental evidence for formation of an interfacial charge-transfer complex between polyheptazine (donor) and TiO$_2$ (acceptor), which is responsible for a significant red shift of absorption and photocurrent response of the hybrid as compared to both of the single components. The direct optical charge transfer from the HOMO of polyheptazine to the conduction band of TiO$_2$ gives rise to an absorption in the visible (2.3 eV; 540 nm). The estimated potential of photogenerated holes (+1.7 V vs. NHE, pH 7) allows for photooxidation of water (+0.82 V vs. NHE, pH 7) through visible light-driven evolution of dioxygen on hybrid electrodes modified with IrO$_2$-Nanopartikeln als Co-Katalysator modifiziert wurde.
Triradikale sind interessante Moleküle, die beispielsweise als Elemente in organischen magnetischen Materialien dienen können. In der Arbeit werden zwei neue Triradikale $1$ und $2$ vorgestellt, die aufgrund ihrer Spin-topologie (Kombination aus einem $\sigma$- und zwei $\pi$-Radikalzentren) von besonderem Interesse sind.

Die beiden Triradikale $1$ und $2$ wurden durch Photolyse der entsprechenden Triiod-Verbindungen in Argonmatrizes erzeugt und durch ESR-Spektroskopie charakterisiert. Übereinstimmend mit Multi-Referenz-Rechnungen nehmen beide Systeme einen Quartett-Grundzustand ein, während beim isomeren Triradikal $3$ der $2\text{B}_2$ Dublett-Zustand energetisch unter dem $4\text{B}_2$ Zustand liegt. Für dieses Triradikal konnte daher unter gleichen experimentellen Bedingungen keines der charakteristischen Quartett-Signale beobachtet werden. Die beste Abschätzung der adiabatischen Dublett-Quartett Energiedifferenz (CAS(7,7)-AQCC/cc-pVTZ//CAS(9,9)-RS2c/cc-pVTZ) bei $1$ - $3$ ergeben sich zu 10.4, 7.7 bzw. 1.3 kcal/mol. Die gemessenen Nullfeldparameter von $1$ und $2$ werden in Hinblick auf die Beiträge der carbenoiden Resonanzstrukturen (Spinpolarisation des $\pi$-Systems) zum Resonanzhybrid der Triradikale diskutiert.

![Triradikale](image1.png)

The isomeric triradicals $1$ and $2$ were generated by irradiation of the corresponding triiodo compounds in cryogenic argon matrices and characterized by EPR spectroscopy. In agreement with multireference computations, both systems possess quartet ground states, whereas in the isomeric triradical $3$ the $2\text{B}_2$ doublet state lies energetically below the $4\text{B}_2$ state. Therefore, no characteristic quartet signals could be observed for this triradical under similar experimental conditions. The best estimates for the adiabatic doublet–quartet energy splittings (CAS(7,7)-AQCC/cc-pVTZ//CAS(9,9)-RS2c/cc-pVTZ) of $1$ – $3$ are 10.4, 7.7, and -1.3 kcal/mol, respectively. The measured zero-field splitting parameters of $1$ and $2$ are discussed in terms of the contributions of carbenoid resonance structures (spin polarization of the $\pi$-system) to the resonance hybrid of the title triradicals.
Gerald Dyker  
Org. Chem. - Organische Synthese und Katalyse;  
Ruhr-Universität Bochum; D-44780 Bochum  
Tel.: ++49-(0)234-3224551; FAX: ++49-(0)234-3214353  
email: Gerald.Dyker@rub.de; http://www.orch.ruhr-uni-bochum.de/dyker/


In the crystalline state multifold alcohol-functionalized chiral calix[4]arenes are forming helical structures with central hydrophilic channel, stabilized by hydrogen bridging bonds. Thereby point chirality is translated into helical homochirality.
The serine/threonine mammalian Sterile 20-like kinase (MST1) is involved in promotion of caspase-dependent and independent apoptosis. The oligomerization domain, denoted as SARAH domain, forms an antiparallel coiled coil dimer and it is important for both, MST1 autophosphorylation and for interactions with other proteins. We show that the monomeric state of SARAH is thermodynamically unstable and that homodimerization is coupled with folding. By investigating the thermal denaturation using differential scanning calorimetry (see figure left) and circular dichroism (see figure right), we have found that the SARAH domain dissociates and unfolds cooperatively, without a stable intermediate monomeric state. The Inhibitory domain is found to be highly flexible and intrinsically unfolded, not only in isolation but also in the dimeric state of the Inhibitory-SARAH construct. More, the Inhibitory domain increases the thermodynamic stability of SARAH monomer and homodimer affinity. These results emphasize the importance of flexibility and binding-induced folding for specificity, affinity and for the capacity to switch from one state to another.

The choice of solvent is crucial for enzyme activity, but obtaining an accurate, quantitative picture of solvent activity during catalysis is quite challenging. Terahertz spectroscopy and X-ray absorption analyses were combined to measure changes in the coupled water-protein motions during peptide hydrolysis of the active centre, the zinc atom of a human metalloprotease. These changes were found to be directly correlated with rearrangements at the active site during the formation of productive enzyme-substrate intermediates and were found to differ from those in an enzyme–inhibitor complex. Molecular dynamics simulations showed a steep gradient of fast-to-slow coupled protein-water motions around the protein, active site and substrate. The results show that water retardation occurs before formation of the functional Michaelis complex. The observed gradient of coupled protein-water motions may assist enzyme-substrate interactions through water-polarizing mechanisms that are remotely mediated by the catalytic metal ion and the enzyme active site.

Structure and function of proteins are predominantly investigated in vitro, in environments ranging from dilute solution to cryogenic crystals. We developed the temperature-jump fluorescence microscope (Fast Relaxation Imaging, FReI) to spatio-temporally resolve fast biomolecular kinetics and stability inside a single living cell. Our recent study focused on mechanistic details of protein folding across the cytoplasm. We show that the general features of cooperative folding transitions and kinetics remain the same as those in vitro, but the folding free-energy landscape and local viscosity vary according to microenvironments in the cellular landscape. Experiments in vitro provide a basis for comparing crowding and chemical effects with experiments inside of the cell. Perhaps cells even evolved to post-translationally modulate protein folding and binding through chemical patterns or by crowding.

Synthetic foldamers such as α/β-, β- and γ-peptides have preferred secondary structures that often extend beyond those found in proteins entirely composed of naturally occurring α-amino acids. Due to the three-carbon bridge between amide groups, γ-peptides offer increased flexibility relative to α-peptides (one carbon) or β-peptides (two carbons). Recent progress in the synthesis of γ-amino acids is leading to an increased effort to understand the folding preferences of γ-peptides. Single-conformation spectroscopy provides the unique opportunity for studies on small γ-peptide oligomers under isolated conditions, where the inherent preferences can be probed in the absence of solvent effects. Such studies provide the natural point of connection with those testing the ability of molecular mechanics force fields or ab initio methods to properly capture the subtle balance of H-bonding, dispersive forces, and steric strain. In the present study, single-conformation IR-UV double-resonance spectroscopy was used to determine the conformer-specific IR spectra of two small γ-peptides, Ac-γ²-hPhe-γ²-hAla-NHMe and Ac-γ²-hAla-γ²-hPhe-NHMe. The single-conformation IR spectra in the NH stretch region reveal that Ac-γ²-hPhe-γ²-hAla-NHMe possesses four conformers, while Ac-γ²-hAla-γ²-hPhe-NHMe possesses three conformers. Four of the seven conformers form C9/C9 sequentially H-bonded double-ring structures, one conformer a C9/C14 bifurcated H-bonded double ring. The remaining two conformers form C7/C7/C14 H-bonded cycles involving all three amide NH groups, a conformation unprecedented in other peptides and peptidomimetics.

Asymmetric catalysis exploits chiral induction by reactants or catalysts, whereas chiral induction by the reaction medium is usually less favorable because the weak solute-solvent coupling leads to low enantioselectivity. Chiral ionic liquids as reaction media with chirality carried by the anion or cation enable more efficient chirality transfer because ions can strongly interact with counter ions and ionic transition states. An intriguing example for chirality transfer between oppositely charged ions is the ruthenium-catalyzed hydrogenation of a keto-functionalized, prochiral imidazolium-based cation in which the chiral camphorsulfonate anion induces chirality at the cation, presumably via ion pairing in the enantioselective reaction step. In collaboration with the group of P. Wasserscheid at the University of Erlangen we could prove this decisive role of ion pairs by dielectric relaxation spectroscopy. We could also show that upon formation of larger ion clusters at high concentrations the defined ion contact necessary for the chirality transfer is lost to a great extent, resulting in a decrease of the enantiomeric excess, as observed experimentally.

Electron-transfer between genetically modified *Hansenula polymorpha* yeast cells and electrode surfaces via Os-complex modified redox polymers

Graphite electrodes, which were modified with redox polymer-entrapped yeast cells were investigated with respect to possible electron transfer pathways between cytosolic redox enzymes and the electrode surface. Either wild-type or genetically modified *Hansenula polymorpha* yeast cells over-expressing flavocytochrome b2 (FC b2) were integrated into Os-complex modified electrodeposition polymers. Upon increasing the L-lactate concentration, an increase in the current was only detected in the case of the genetically modified cells. The overexpression of FC b2 and the related amplification of the FC b2/L-lactate reaction cycle was found to be necessary to provide sufficient charge to the electron-exchange network in order to facilitate sufficient electrochemical coupling between the cells, via the redox polymer, to the electrode. The close contact of the Os-complex modified polymer to the cell wall appeared to be a prerequisite for electrically wiring the cytosolic FC b2/L-lactate redox activity and suggests the critical involvement of a plasma membrane redox system. Insights in the functioning of whole-cell based bioelectrochemical systems have to be considered for the successful design of whole-cell biosensors or microbial biofuel cells.


Until recently, rhodium(III) and particularly iridium(III) compounds were generally considered as being unlikely prospective candidates for anticancer agents owing to their typical kinetic inertness. Our systematic studies on the cellular impact of their octahedral polypyridyl complexes have, however, demonstrated that high cytotoxicity towards human cancer cells and in certain cases associated relative tolerance by healthy cells can be achieved by judicious selection of the remaining ligands. fac-\([\text{IrCl}_3(\text{DMSO})(5,6-\text{Me}_2\text{phen})]\), for instance, exhibits a significant selectivity for both adhesive and non-adhesive malignant cells. Selectivity can be further significantly enhanced for the much more potent meridional rhodium(III) complexes by introducing 5-Cl or 5-\(\text{NO}_2\) substituents into the phenanthroline ligand. As a response to oxidative stress signalling, these trichlorido complexes cause an immediate decrease in the respiration of MCF-7 breast cancer cells, followed by a time-delayed induction of apoptosis by an intrinsic mitochondrial pathway.

We present a simple, time- and cost-efficient approach to tackle the proteome of prokaryotic organisms. To obtain large data sets of complex biological experiments high-throughput and time- and cost-efficient methods still have to be developed and refined. In this study, we combined well-approved techniques, namely elevated chromatographic temperatures, long RP columns and the multidimensional protein identification technology MudPIT to achieve high proteome coverage. The advanced MudPIT approach has been evaluated and delivered very comprehensive results for Gram-positive as well as Gram-negative bacteria (53% proteome coverage for Corynebacterium glutamicum and 46% proteome coverage for Escherichia coli). Also, a high identification rate for the challenging integral membrane proteins was achieved. The competitiveness of the advanced MudPIT technology is strengthened by the fact that in this approach only two fractions were analyzed with both, simple and time efficient sample preparation, and a moderate data acquisition time.

Here we demonstrate an electrochemical device called “mixing entropy battery”, which can extract the wasted entropic energy derived from salinity gradient and transform it directly to electric energy, allowing renewable production of electricity. This battery can be applied to extract energy from the salinity difference between sea and river water. For the demonstration of the working principle, the mixing entropy battery was built by using a cation capturing electrode based on nanostructured Na$_2$Mn$_5$O$_{10}$ and an anion capturing electrode based on silver. The battery showed energy extraction efficiency up to 74%. By means of impedance spectroscopy it was possible to separate the contribution of the single elements of the device to the total overvoltage. It was possible to individuate high overpotentials connected with the formation and thickening of the AgCl layer on the Ag electrode during the capturing of the chloride ions. Also the diluted fresh water solution has shown to introduce high potential drops. An optimization process would be possible, and it is predicted that efficiencies up to 83% should be possible. Considering the flow rate of river water into ocean as the limiting factor, our calculations of potential energy production indicate that the total generated renewable energy could reach 2 TW, or ~13% of the current world energy consumption.
Simultaneous acquisition of electrochemical impedance spectroscopy and quartz crystal microbalance (EIS-EQCM) data in cyclic electrode potential scans was used to characterize nonstationary underpotential deposition (UPD) of atomic layers of Ag on Au and Cu on Pt. Both EIS and EQCM data sets complemented each other in the elucidation of interface models and the investigation of different aspects of the interfacial dynamics. EIS-EQCM provided an opportunity to monitor coadsorption and competitive adsorption of anions during the Ag and Cu UPD using (i) the electrode mass change, (ii) adsorption capacitances, and (iii) double-layer capacitances. Kinetic information is available in the EIS-EQCM through the charge transfer resistances and apparent rate coefficients. The latter expresses the rate of UPD into the partially covered electrode surface. The EIS-EQCM appeared to be a promising tool for an improved characterization and understanding of nonstationary electrochemical interfaces.

Nuclear quantum effects on the structure of dissociated HCl(H₂O)₄ clusters are studied using ab initio path integral simulations. This cluster supports two distinct zwitterionic species serving as minimal microsolvation models for solvent-shared and contact ion pairs. The structure of the contact ion pair is qualitatively changed due to nuclear quantum effects: the hydrogen bond that directly connects the ion pair becomes both centered and fluxional as a result of zero point motion. This so-called "low-barrier hydrogen bonding" scenario is relevant to bulk acid dissociation ultra-high concentrations.
Graphite and diamond have comparable free energies, yet forming diamond from graphite in the absence of a catalyst requires pressures that are significantly higher than those at equilibrium coexistence. At lower temperatures, the formation of the metastable hexagonal polymorph of diamond is favoured instead of the more stable cubic diamond. These phenomena cannot be explained by the concerted mechanism suggested in previous theoretical studies. Using an ab initio quality neural-network potential, we carried out a large-scale study of the graphite-to-diamond transition assuming that it occurs through nucleation. The nucleation mechanism accounts for the observed phenomenology and reveals its microscopic origins. We demonstrate that the large lattice distortions that accompany the formation of diamond nuclei inhibit the phase transition at low pressure, and direct it towards the hexagonal diamond phase at higher pressure. The proposed nucleation mechanism should improve our understanding of structural transformations in a wide range of carbon-based materials.

An implementation of scaled opposite-spin CC2 (SOS-CC2) for ground and excited state energies is presented, that requires only fourth order scaling computational costs. The SOS-CC2 method yields results with an accuracy comparable to the unscaled method. Furthermore the time-determining fifth order scaling steps in the algorithm can be replaced by only fourth order scaling computational costs using a ``resolution of the identity'' approximation for the electron repulsion integrals and a Laplace transformation of the orbital energy denominators. This leads to a significant reduction of computational costs especially for large systems. Timings for ground and excited state calculations are shown and the error of the Laplace transformation is investigated. An application to a chlorophyll molecule with 134 atoms results in a speed-up by a factor of five and demonstrates how the new implementation extends the applicability of the method. A SOS variant of the algebraic diagrammatic construction through second order ADC(2), which arises from a simplification of the SOS-CC2 model, is also presented. The SOS-ADC(2) model is a cost-efficient alternative in particular for future extensions to spectral intensities and excited state structure optimizations.
Werner Kutzelnigg
Theoretische Chemie; Ruhr-Universität Bochum; D-447780 Bochum
Tel.: ++49-(0)234-3226200; FAX: ++49-(0)234-3214109
e-mail: Werner.Kutzelnigg@rub.de
http://www.theochem.ruhr-uni-bochum.de/research/kutzelnigg/


A hierarchy of approximations in relativistic many-electron theory is discussed that starts with the Dirac equation and its expansion in a kinetically balanced basis, via a formulation of non-interacting electrons in Fock space (which is the only consistent way to deal with negative-energy states). The most straightforward approximate Hamiltonian for interacting electrons is derived from quantum electrodynamics (QED) in Coulomb gauge with the neglect of transversal photons. This allows an exact (non-perturbative) decoupling of the electromagnetic field from the fermionic field. The electric interaction of the fermions is non-retarded and non-quantized. The quantization of the fermionic field leads to a polarizable vacuum. The simplest (but somewhat problematic) approximation is a no-pair projected theory with external-field projectors. The Dirac Coulomb operator in configuration space (first quantization) is not acceptable, even if the Brown-Ravenhall disease is much less virulent than often claimed. Effects of transversal photons, such as the Breit interaction and renormalized self-interaction can be taken care of perturbatively at the end, but there are still many open questions.
An accurate calculation of adsorption energies for small molecules on solid surfaces is possible with wave function based quantum chemical \textit{ab initio} methods, even in the case of weak van der Waals interactions, but such calculations are extremely time consuming. The method of “local increments”, where the total interaction is decomposed into a sum of one-body, two-body and higher increments, leads to a strong reduction of the necessary computer time without loss of accuracy and allows for a simple physical interpretation of the different contributions to the total interaction energy: Pauli (SCF) repulsion, van der Waals attraction (dispersion), modification of the partners by the interaction. By means of this approach, we could calculate for the first time a reliable potential energy curve for the adsorption of CO on the MgO(001) surface without using semiempirical parameters.
In this paper, for the first time an investigation into the dependence of the accuracy of activity coefficients at infinite dilution, calculated from the conductor-like screening model for real solvents (COSMO-RS), on the basis set and the quantum chemical method used. Activity coefficients at various temperatures serve as experimental parameters for optimising the COSMO-RS parameters. A modification of the energy function of COSMO-RS is presented; this leads to a higher accuracy of parameterisation. When using density functional theory, at least a valence double-zeta basis set is necessary for good accuracy. Interestingly, for all the investigated functionals, larger basis sets show no advantages. The most accurate parameterisation was obtained with MP2.

The Fischer-Tropsch synthesis (FTS) is a well-established industrial process for converting synthesis gas (CO, H₂) into mainly linear hydrocarbons with a broad carbon number distribution. The industrial FTS process is often performed using iron catalysts promoted with copper or potassium in order to improve its CO dissociation properties. As the dissociation of CO is one of the key steps the kinetics and thermodynamics of CO adsorption/dissociation were systematically investigated. Using a combination of different analytical methods it was shown that the Fe-C bond was strengthened in the presence of potassium leading to a facilitated CO dissociation. Furthermore potassium promotion led to a blocking of high-energy adsorption sites on the catalyst surface, thus changing its energy distribution.
A model version of the highly active Au/TiO$_2$ catalyst system was made by inserting both components into a mesoporous MCM-48 matrix in order to enforce high dispersion on both metal (Au) and support (TiO$_2$). In CO oxidation, activities achieved were comparable with those of real catalysts. The TiK EXAFS spectrum proved to be completely invariant notwithstanding great variations in the state of gold (figure), which shows that high activity does not require an ordered (epitactic) relation between metal and support. From the average Au particle size being below 1 nm it was concluded that the metal-non metal transition is irrelevant for the activity of gold. During activation of the model catalysts in the feed, significant poisoning phenomena (probably by carbonate) were observed. Such poisoning is much less pronounced with real catalyst, which suggests that the much larger TiO$_2$ surface of real catalysts protects the active Au-TiO$_2$ perimeter by trapping and storing poisonous adsorbates.
Anorganische Füllmaterialien dienen oft der Verbesserung der mechanischen, thermischen und chemischen Eigenschaften von Polymermembranen. Im Falle protonenleitender Polymere ist es dabei allerdings gleichzeitig nötig, die Protonenleitung der Matrix zu unterstützen bzw. wenigstens nicht zu stören. Durch geeignete Kombinationen aus Polymer und Füllermaterial können so effektive und sehr gut leitfähige Kompositmembranen hergestellt werden. Dieser Artikel gibt einen Überblick über die möglichen Anwendungen einer speziellen Form derartiger protonenleitender Kompositmembranen, die funktionalisierte SiO₂-Partikel mit geordneter Mesoporosität enthält, in Brennstoffzellen, zur Entsalzung von Wasser und in der Photokatalyse.

Insbesondere in dem hochaktuellen Themengebiet der photokatalytischen Wasserspaltung finden diese Kompositmembranen eine wichtige Anwendung: So wird die Konstruktion einer 2-Kammer Zelle beschrieben, mit der es durch Einsatz besagter Membranen möglich wird, Wasserstoff und Sauerstoff räumlich getrennt voneinander zu generieren, so dass hohe Kosten für nachträgliche Gastrennung und –aufreinigung gespart werden können. Außerdem wird in diesem Zusammenhang gezeigt, dass die Menge an funktionalisierten mesoporösen SiO₂-Partikeln ein wichtiger Faktor in der Protonenleitfähigkeit der Komposite ist.

Inorganic filler materials are often incorporated into polymer membranes to improve their mechanical, thermal and chemical stabilities. In case of proton-conducting polymers, however, it is necessary to support or at least not to disturb the proton-conducting matrix. By suitable combination of polymer and filler, effective and highly conductive composite membranes can be prepared. This article gives an overview of the possible applications of a special kind of such proton-conducting composite membranes containing functionalised SiO₂ particles with ordered mesoporosity in fuel cells, in desalination and in photocatalysis. Particularly, these composite membranes find an important application in the highly active area of the photocatalytic water splitting: Thus, in the article, the construction of a 2-compartment cell is described with which it is possible by use of the mentioned membranes to generate hydrogen and oxygen spatially separated from each other, so that high costs for subsequent gas separation and purification can be saved. Additionally, it is also shown in this context that the amount of functionalized mesoporous SiO₂ particles is a major factor in the proton conductivity of the composites.
A combined experimental and first principles study of Cu defects in bulk ZnO is presented. Cu particles are epitaxially deposited on the polar O-ZnO(000 1) surface at RT. Upon heating, a broadening of the quasi-elastic peak in high resolution electron energy loss spectra is observed, corresponding to an electronic doping effect of Cu atoms in bulk ZnO with an ionization energy of 88 meV. Cu impurities in ZnO, although commonly acting as acceptors, are presently observed to induce shallow donor states. We assign these to interstitial Cu⁺ species on the basis of a hybrid density functional study.
Jennifer Strunk  
Lehrstuhl für Technische Chemie; Ruhr-Universität Bochum; D-44780 Bochum  
Tel.: ++49-(0)234-3223566; FAX: ++49-(0)234-3214115  
email: jennifer.strunk@techem.rub.de; http://www.techem.ruhr-uni-bochum.de


Für Übergangsmetalle wie zum Beispiel TiO$_2$ und V$_2$O$_5$ existieren bereits gut etablierte Prozesse, um (Sub)Monolagen auf inerte Träger aufzubringen. Bei geringen Bedeckungen werden so durch die M-O-Si-Bindungen neue aktive Zentren gebildet, während bei hohen Bedeckungen die Eigenschaften des katalytisch aktiven Oxids mit der großen Oberfläche des inerten Trägers kombiniert werden. Für das einfach reduzierbare Seltenerdoxid CeO$_2$ sind bisher keine Studien veröffentlicht worden, in denen Schichten erfolgreich synthetisiert und umfassend charakterisiert wurden. In der vorliegenden Arbeit wurde der Einfluss der Art des Präkursors und der Synthesemethode auf die Struktur der abgeschiedenen Cerioxidepezies untersucht. Einheitliche Cerioxidnanopartikel mit einem Durchmesser von 3 nm wurden erhalten, wenn Ceracetylacetonat auf SiO$_2$ gegraft wurde. Schichtartige Strukturen konnten erfolgreich synthetisiert werden, wenn Cer-tert.-butoxid verwendet wurde. Die Reduzierbarkeit der beiden strukturell unterschiedlichen Cerioxidepezies ist identisch, aber im Fall der Schichten wird die Reduktion partiell irreversibel, wenn sie bei 923 K durchgeführt wird. Dieser Effekt könnte der Bildung von Cersilikaten zugeschrieben sein, welche die Reoxidation des Cers verhindern. Im Fall der Nanopartikel ist die Reduktion komplett reversibel.

For transition metal oxides such as TiO$_2$ or V$_2$O$_5$ well-established processes exist to support (sub)monolayers on inert supports. At low coverage new active sites due to M-O-Si bonds are created, and at high coverage the properties of the catalytically active oxide are combined with the large surface area of the inert support. For the easily reducible rare earth oxide CeO$_2$, no previous studies have been published in which layers were successfully prepared and thoroughly characterized. In the present work, the effect of the nature of the precursor and the synthesis method on the structure of the deposited ceria species has been evaluated. Uniform ceria nanoparticles with a diameter of 3 nm have been obtained by grafting cerium acetylacetonate on silica. Layer-like species could be successfully synthesized when using cerium tert.-butoxide. The reducibility of both structurally different ceria species is similar, however, in case of the layers, when reduction is carried out at 923 K, it becomes partially irreversible. This effect might be attributed to the formation of cerium silicates that prevent reoxidation of cerium. In case of the nanoparticles reduction is fully reversible.

The computational power of the human brain results from the complexity of the myriad interactions of its roughly 100 billion nerve cells which, on average, make 7000 contacts with other neurons. This largely unexplained complex network is clearly based upon the electrical activity of the participating neurons, which in turn is dependent on the neurotransmitter receptors that receive signals from other neurons. Glutamate receptors, the most widely expressed group of neurotransmitter receptors, play a very special role in this signaling. This is why understanding the structural diversity that underlies their functional variability is essential. In our study we analyzed the connection between glutamate receptor variants and dendritic tree morphology of some 16,000 neurons and found that, depending on the type of neuron, different receptor subunits trigger dendritogenesis. In interneurons (Fig. A), GluA1(Q)-flip is the sole effective subunit, while in pyramidal neurons (Fig. B) GluA2(R)-flip, GluA2(Q)-flip, GluA2(Q)-flop and GluA3(Q)-flip serve that role. The common denominator of the latter four subunits is their slow desensitization, which leads to increased calcium influx that ultimately triggers dendritogenesis.

Accessory β-subunits of the KCNE gene family modulate the function of various cation channel α-subunits by the formation of heteromultimers. Among the most dramatic changes of biophysical properties of a voltage gated channel by KCNEs are the effects of KCNE1 on Kv7.1 channels. Kv7.1 and KCNE1 are believed to form native $I_{Ks}$ channels. Here, we characterize molecular determinants of KCNE1 interaction with Kv7.1 channels by scanning mutagenesis, double mutant cycle analysis, and molecular dynamics simulations. Our findings suggest that KCNE1 binds to the outer face of the Kv7.1 channel pore domain, modifies interactions between voltage sensor, S4-S5 linker and the pore domain, leading to structural modifications of the selectivity filter and voltage sensor domain. Molecular dynamics simulations suggest a stable interaction of the KCNE1 transmembrane α-helix with the pore domain S5/S6 and part of the voltage sensor domain S4 of Kv7.1 in a putative pre-open channel state. Formation of this state may induce slow activation gating, the pivotal characteristic of native cardiac $I_{Ks}$ channels. This new Kv7.1-KCNE1 model may become useful for dynamic modeling of disease associated mutant $I_{Ks}$ channels.


Our studies suggest that the genetic enhancement of H-Ras-MAPkinase signaling in adult neurons affects the generation and dendritic differentiation of newborn cells within the adult hippocampus. Neurogenesis is down-regulated at an early stage of the proliferative cascade altering the pool of young highly plastic cells that are critical for hippocampus-dependent learning and memory. Accordingly, synRas mice display impairments in spatial short-term memory and object recognition. Neurogenesis as well as object recognition can be restored by voluntary exercise supporting a link between neurogenesis and hippocampus-dependent cognition. Young neurons might be necessary especially under conditions requiring increasing demands to associate stimuli over time and/or space.

The presence of the membrane lipid phosphatidylcholine (PC) in the bacterial membrane is critically important for many host-microbe interactions. The phospholipid N-methyltransferase PmtA from the plant pathogen Agrobacterium tumefaciens catalyzes the formation of PC by a three-step methylation of phosphatidylethanolamine via monomethylphosphatidylethanolamine and dimethylphosphatidylethanolamine. The methyl group is provided by S-adenosylmethionine (SAM), which is converted to S-adenosylhomocysteine (SAH) during transmethylation. Despite the biological importance of bacterial phospholipid N-methyltransferases, little is known about amino acids critical for binding to SAM or phospholipids and catalysis. Alanine substitutions in the predicted SAM-binding residues E58, G60, G62, and E84 in A. tumefaciens PmtA dramatically reduced SAM-binding and enzyme activity. Homology modeling of PmtA satisfactorily explained the mutational results. The enzyme is predicted to exhibit a consensus topology of the SAM-binding fold consistent with cofactor interaction as seen with most structurally characterized SAM-methyltransferases. Nuclear magnetic resonance (NMR) titration experiments and 14C-SAM-binding studies revealed binding constants for SAM and SAH in the low micromolar range. Our study provides first insights into structural features and SAM binding of a bacterial phospholipid N-methyltransferase.
In this article, we describe a simple, reliable, and inexpensive procedure to qualitatively demonstrate the antioxidative capacity using the well-discussed and impressive chemoluminescence reaction of lightsticks. When a lightstick is snapped, it shows a bright chemoluminescence. This luminescence results from the reaction of the hydrogen peroxide (from the glass vial in the lightstick) with the phenyl oxalate ester (in the plastic tube). After the addition of the test substance (= antioxidant ingredients, e.g., ascorbic acid or flavonoids such as naringin), the light intensity of the batch shows an obvious decay compared to the blank test, which shows the normal luminescence of a lightstick (Figure 1). The observed decay of the light intensity after the addition of the assay can be traced back to its antioxidative capacity.

Bioorganometallic Chemistry is a young and interdisciplinary field of study. This Research Unit ("Forschergruppe") will establish organometallic chemistry as part of medicinal chemistry. Funding for this Research Unit by the German Funding Agency (DFG) started in 2006 and is expected to run until the middle of 2012. Selected classes of organometallic compounds will be studied in their interaction with cellular components like receptors, proteins, peptides and DNA. We are aiming to identify metal-specific mechanisms of cytotoxicity. The findings will guide the design of novel metal-based lead structures and contribute to the understanding of signalling pathways and protein expression patterns. In 2011, more than ten joint papers were published from this Research Unit. Progress in this Research Unit will contribute to the development of medicinal bioorganometallic chemistry in Germany and beyond. Funding of FOR 630 will end in 2012.

After its foundation in October 2009 CES is now completed and fully operational. The core of CES is a central electrochemistry laboratory equipped with modern electrochemical-, microscopic- and spectroscopic techniques. The research groups of the two speakers supported by three junior research groups “Molecular Nanostructures” (Dr. Nicolas Plumere), “Semiconductor Electrochemistry and Energy Conversion“ (Dr. Fabio La Mantia) and “Adsorption and Electrocatalysis” (Dr. Aliaksandr Bandarenka) work together with 15 post-docs, 11 PhD students and several master students on a broad range of electrochemical topics like Li-ion-batteries, semiconductors, photoelectrochemistry, photoelectrochemical water splitting, catalysts for oxygen reduction/oxidation, fuel cells, and biosensors. The experimental studies are completed by development of new sophisticated electrochemical methods as well as theoretical electrochemistry. The results of the scientific studies have already been presented on various national and international conferences and are published in more than 20 peer-reviewed scientific papers.

Im August 2011 hat Prof. Dr. M. Havenith-Newen ihre Sprecherinfunktion an Prof. A.-V. Mudring übergeben. Als neue Mitglieder wurden in 2011 folgende Wissenschaftler aufgenommen: Prof. Dr. K. Morgenstern, Prof. Dr. M. Wark, JP Dr. R. Beránek, JP Dr. S. Ebbinghaus, Dr. Ch. Müller, Dr. N. Plumeré, Dr. F. La Mantia, Dr. A. Bandarenka, Dr. S. Kareth und Dr. J. Strunk. Mit der Aufnahme von 8 Nachwuchswissenschaftlern/innen zeigt das RD IFSC ganz klar, dass die Förderung von jungen Wissenschaftlern/innen höchste Priorität hat. Das Department Management hat Dr. S. Borgmann im März 2011 übernommen und unterstützt so auch den neuen Masterstudienangang „Molecular Sciences and Simulation“ (www.rub.de/imos). Das IFSC Praktikum wurde optimiert und koordiniert von Prof. A. Devi.


2001 the Research Department Interfacial Systems Chemistry (RD IFSC) has focussed on establishing large collaborative projects. A milestone was the full proposal for a new research building, ZEMOS, a centre for molecular spectroscopy and simulation of solvent-directed processes (www.rub.de/zemos) which was positively evaluated by the German Research Council and now receives 44 Mio. € funding. The RD IFSC also supported the RUB participation in the excellence initiative such as in the excellence cluster „RESOLV“ which is occupied with investigating solvation processes in chemistry, biochemistry and engineering sciences (Solvation Science, www.rub.de/solvation). Together with the other RUB Research Departments the RD IFSC has become an integral part of the Research Campus RUB in bringing researchers and their activites together across scientific disciplines and faculties.

The success of the RD IFSC is documented by the more than 100 publications in peer-reviewed journals of its members. 15 awards were received by established RD members and 10 new numbers, amongst them 8 young talents, were elected as new members.
ZEMOS
Zentrum für Molekulare Spektroskopie und Simulation solvensgesteuerter Prozesse
Sprecherin: Martina Havenith


Mit dem Forschungsbau ZEMOS wird ein national einzigartiges und international herausragendes Zentrum für Solvation Science an der RUB errichtet werden. Forscher der Ruhr-Universität Bochum (RUB) sowie der Max-Planck-Institute (MPI) für Kohlenforschung (Mülheim/Ruhr) und für Eisenforschung (Düsseldorf) nehmen auf diesem Gebiet eine internationale Spitzenposition ein. Der Forschungsbau dient dazu, diesen Vorsprung gezielt weiter auszubauen und Möglichkeiten zu schaffen, die über die jetzt in den einzelnen Arbeitsgruppen verfügbaren weit hinausgehen. Im Zuge einer strategischen Ausrichtung der RUB werden daher folgende Schritte unternommen: 1. Es werden 4 Professuren für die Forschung im Bereich Solvation Science eingerichtet, für die erst mit dem Forschungsbau ZEMOS die erforderlichen Arbeitsbedingungen geschaffen werden. 2. Als direkte Schnittstelle zwischen Grundlagenforschung und technischer Anwendung im Bereich Solvation Science wurden zwei neue Zentren an der RUB eingerichtet: das Center of Electrochemical Sciences (CES) und das Applied Competence Center Terahertz (ACC THz). 3. ZEMOS dient gezielt dazu, die Nachwuchsförderung im Bereich Solvation Science weiter auszubauen.
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