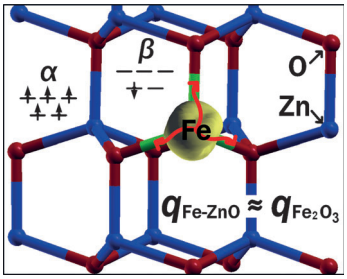
Nanoparticles

J. Xiao, A. Kuc, S. Pokhrel, L. Mädler, R. Pöttgen, F. Winter, T. Frauenheim, T. Heine*

Fe-Doped ZnO Nanoparticles: The Oxidation Number and Local Charge on Iron, Studied by ^{57}Fe Mößbauer Spectroscopy and DFT Calculations

Iron bru: Fe-doped ZnO may contain Fe^{2+} and Fe^{3+} species. Whilst Mößbauer spectroscopy can distinguish these sites in pure oxides FeO and Fe_2O_3, it gives very similar shifts for Fe-doped phases. This result is rationalized by electron redistribution from the dopant site to the crystal matrix. Mößbauer shifts correlate with the local charge on the Fe sites and different dopant sites can be identified by the Mößbauer quadrupole splitting (see figure).



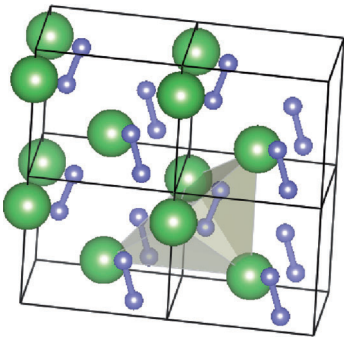
Chem. Eur. J.
DOI: **10.1002/chem.201204308**

Pernitrides

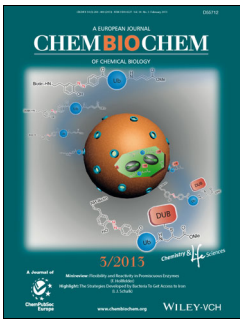
A. Kulkarni, J. C. Schön,* K. Doll, M. Jansen

Structure Prediction of Binary Pernitride MN_2 Compounds (M = Ca, Sr, Ba, La, and Ti)

It's raining MN_2: The energy landscapes of pernitrides of metals with different maximum valence (M = Ca, Sr, Ba, La, and Ti) were globally explored and trends in their structural, physical, and electronic properties were investigated. For TiN_2, a new structure type, TiN_2-I, was found to constitute the thermodynamically stable modification.



Chem. Asian J.
DOI: **10.1002/asia.201200794**

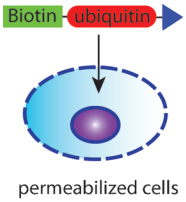


Ubiquitins

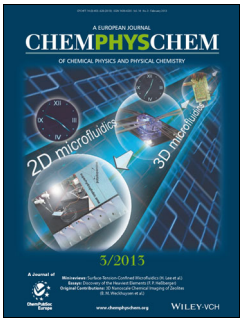
J. H. L. Claessen, M. D. Witte, N. C. Yoder, A. Y. Zhu, E. Spooner, H. L. Ploegh*

Catch-and-Release Probes Applied to Semi-Intact Cells Reveal Ubiquitin-Specific Protease Expression in *Chlamydia trachomatis* Infection

Lifting the cloak: Equipping activity-based probes for deubiquitylating enzymes (DUBs) with catch-and-release handles and subsequent delivery of these probes to the cytosol of semi-intact cells allows the study of deubiquitylating enzymes under conditions as close to physiological as possible. Using these conditions, we demonstrated that the second chlamydial DUB is expressed during the course of infection.



ChemBioChem
DOI: **10.1002/cbic.201200701**

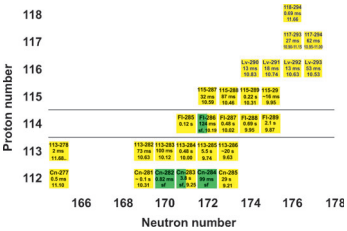


Nuclear Physics

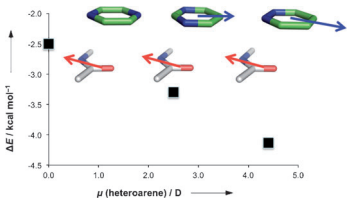
F. P. Heßberger*

Discovery of the Heaviest Elements

Still haven't (quite) found what I'm looking for: The search for new superheavy elements is at present one of the most exciting adventures in nuclear physics. Thanks to enhanced experimental techniques, the synthesis of elements $Z = 113$ to 118 in reactions using ^{48}Ca projectiles and targets made of isotopes of the elements neptunium to californium has been claimed.



ChemPhysChem
DOI: **10.1002/cphc.201201011**



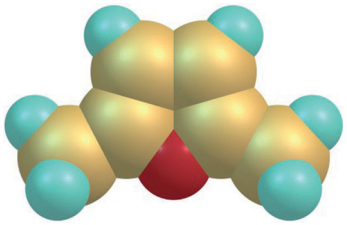
ChemMedChem
DOI: **10.1002/cmdc.201200512**

Drug Design

M. Harder, B. Kuhn,* F. Diederich*

Efficient Stacking on Protein Amide Fragments

π-Stacking: Quantum chemical calculations and Protein Data Bank searches on *N*-methylacetamide/heteroarene stacking were performed, yielding new guidelines that will help future structure-based drug design. The stacking interaction depends on the relative orientation and the magnitude of the two dipole moments, as well as the π-electron density of the arene.



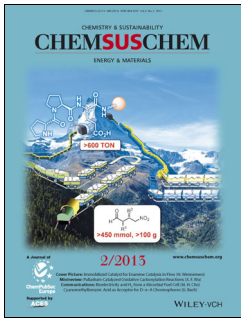
ChemSusChem
DOI: **10.1002/cssc.201200738**

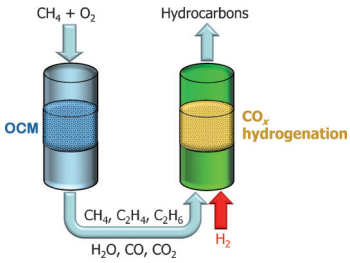
Biofuels

J. M. Simmie,* J. Würmel

Harmonising Production, Properties and Environmental Consequences of Liquid Transport Fuels from Biomass—2,5-Dimethylfuran as a Case Study

Fuel for the future? 2,5-Dimethylfuran has been the subject of many recent studies since its potential as a 'green next-generation' biofuel was highlighted in 2007. The chemistry of this compound is characterised by unusually strong ring-carbon-to-hydrogen bonds, and some of its derivatives are distinguished by extremely weak bonds. This combination makes the task of unravelling their chemistry, and the impacts on the environment and human health, both interesting and challenging.





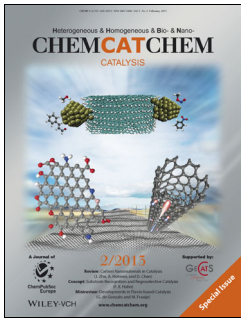
ChemCatChem
DOI: **10.1002/cctc.201200779**

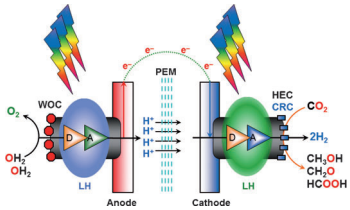
Selective Conversion

E. V. Kondratenko,* U. Rodemerck

A Dual-Reactor Concept for the High-Yielding Conversion of Methane into Higher Hydrocarbons

Dual to the death: The selective conversion of methane into higher alkanes in industrially relevant conversions combines the oxidative coupling of methane (OCM) with the selective hydrogenation of CO and CO_2 in a second reactor, without the need for expensive pre-separation of the reaction products that are formed in the OCM reactor. Thus, the yield of higher alkanes (34%) is at least 50% higher than that from a single OCM reactor.





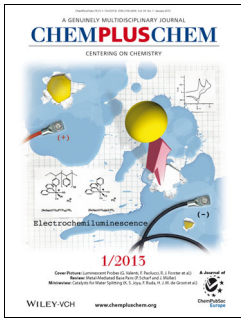
ChemPlusChem
DOI: **10.1002/cplu.201200161**

Catalysts for Water Splitting

K. S. Joya,* J. L. Vallés-Pardo, Y. F. Joya, T. Eisenmayer, B. Thomas, F. Buda,* H. J. M. de Groot*

Molecular Catalytic Assemblies for Electrodriven Water Splitting

Splitting up: An overview of molecular catalytic assemblies for electrochemical water oxidation and an analysis of recent progress in catalyst design and performance are presented, including systems integration of modules for future stand-alone solar-to-fuel conversion devices (see figure). The thermodynamics of intermediates and the mechanism of O–O bond formation are also described.

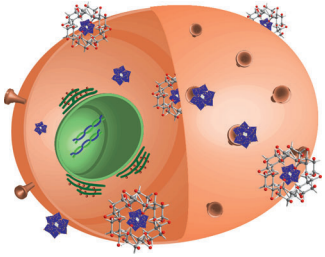


Enzyme Inhibition

H. Stephan,* M. Kubeil, F. Emmerling, C. E. Müller*

Polyoxometalates as Versatile Enzyme Inhibitors

Polyoxometalates (POMs) are metal cluster compounds with a broad range of pharmacological properties, including antidiabetic, antibacterial, antiprotozoal, antiviral and anticancer activities. The inhibition of enzymes, in particular those accessible from the extracellular space, may constitute an important biological mechanism of action of POMs.



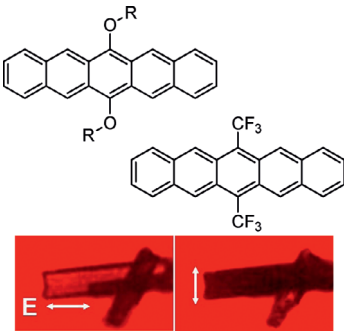
Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.201201224**

Functional Materials

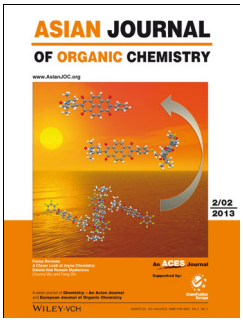
J. Schwaben, N. Münster, T. Breuer, M. Klues, K. Harms, G. Witte, U. Koert*

Synthesis and Solid-State Structures of 6,13-Bis(trifluoromethyl)- and 6,13-Dialkoxypentacene

The electrochemical and optical properties of 6,13-disubstituted pentacenes, in addition to their solid-state packing motifs, were determined. 6,13-Bis(trifluoromethyl)pentacene and 6,13-dimethoxypentacene exhibit slipped face-to-face π stacking in the solid state, whereas 6,13-diethoxypentacene forms pairs of π-stacking molecules in the solid state.



Eur. J. Org. Chem.
DOI: **10.1002/ejoc.201201714**

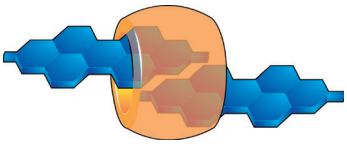


Cucurbit[8]uril Binding

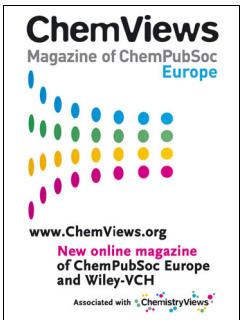
K. J. Hartlieb, A. N. Basuray, C. Ke, A. A. Sarjeant, H.-P. Jacquot de Rouville, T. Kikuchi, R. S. Forgan, J. W. Kurutz, J. F. Stoddart*

Chameleonic Binding of the Dimethyldiazaperopyrenium Dication by Cucurbit[8]uril

Two are better than one: The diazaperopyrenium dication acts as both a viologen-like electron-poor and an electron-rich guest, resulting in the formation of a 1:2 complex with cucurbit[8]uril. This chameleonic binding facilitates deaggregation of the dications from aqueous solutions, leading to an increase in the fluorescence quantum yield of the diazaperopyrenium dication.



Asian J. Org. Chem.
DOI: **10.1002/ajoc.201200187**



Energy Technology

S. Watson

Tomas Kåberger on Global Energy Industry

Professor Tomas Kåberger is an expert of science, economics, and politics of the global energy industry with broad experience in Europe and Asia. He talks about the current trends and challenges of the global energy industry, including how the biggest challenge may not be developing technology, but in the murky problem of removing institutional barriers.

ChemViews magazine
DOI: **10.1002/chemv.201300007**