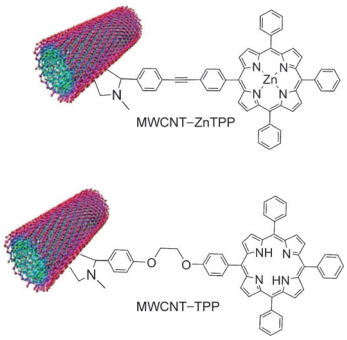
Nanohybrids

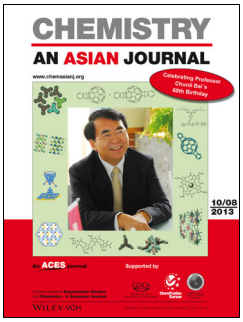
A. Wang, Y. Fang, L. Long, Y. Song, W. Yu, W. Zhao, M. P. Cifuentes, M. G. Humphrey, C. Zhang*

Facile Synthesis and Enhanced Nonlinear Optical Properties of Porphyrin-Functionalized Multi-Walled Carbon Nanotubes

Enhanced nonlinear properties: Two porphyrin-functionalized multi-walled carbon nanotubes (MWCNTs) were constructed by facile 1,3-dipolar cycloaddition reactions. Covalent attachment of the porphyrin moieties to the surface of the MWCNTs significantly improves their solubility and processability. The enhanced optical nonlinearities were observed for such porphyrin-functionalized MWCNT nanohybrids, which can be attributed to the covalent linkage between the porphyrin and the MWCNTs.



Chem. Eur. J.
DOI: **10.1002/chem.201302477**

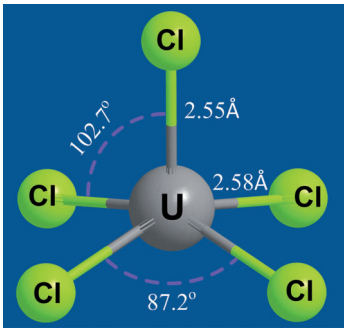


Photoelectron Spectroscopy

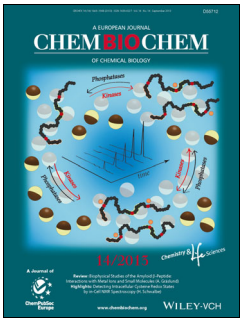
J. Su, P. D. Dau, C.-F. Xu, D.-L. Huang, H.-T. Liu, F. Wei, L.-S. Wang,* J. Li*

A Joint Photoelectron Spectroscopy and Theoretical Study on the Electronic Structure of UCl_5^- and UCl_5

U complete me: Photoelectron spectroscopy and relativistic quantum chemistry calculations were combined to probe the electronic stabilities and electronic structures of the uranium pentachloride complex. The photoelectron spectra were interpreted with the theoretical results, and the bonding interactions between U and Cl were analyzed. The periodic trend for all the UX_5^- (X = F, Cl, Br, and I) series was also investigated.



Chem. Asian J.
DOI: **10.1002/asia.201300627**

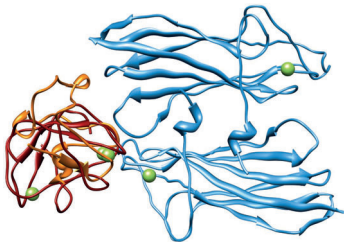


Electron-Transfer Complexes

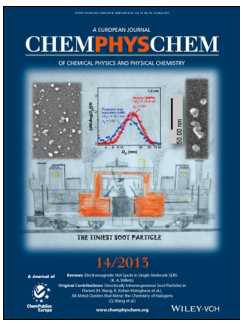
R. M. Almeida, P. Turano, I. Moura, J. J. G. Moura, S. R. Pauleta*

Superoxide Reductase: Different Interaction Modes with its Two Redox Partners

One way or another: Superoxide reductase is used by anaerobic bacteria to detoxify reactive oxygen species, reducing $O_2^{\bullet-}$ to H_2O_2 without producing molecular oxygen. The interaction of superoxide reductase from *Desulfovibrio gigas* with electron donors rubredoxin and desulforedoxin was characterized by using steady-state kinetics, 2D NMR titrations, and backbone relaxation measurements.



ChemBioChem
DOI: **10.1002/cbic.201300196**

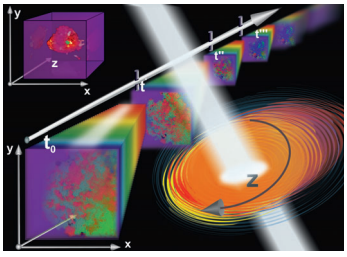


Nanoimaging

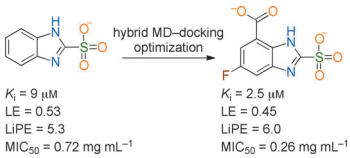
J. C. Andrews,* B. M. Weckhuysen*

Hard X-ray Spectroscopic Nano-Imaging of Hierarchical Functional Materials at Work

Big brother is X-raying you: Full-field hard X-ray spectroscopic nano-imaging is a powerful method to obtain single-pixel chemistry of hierarchical functional materials, such as catalytic solids, fuel cells, and batteries, during operation at realistic temperatures and pressures and with around 30 nm spatial resolution. Some technical aspects, as well as recent showcases, and future perspectives on the application of this characterization tool are presented.



ChemPhysChem
DOI: **10.1002/cphc.201300529**



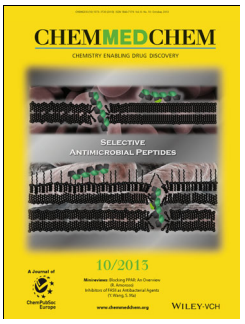
ChemMedChem
DOI: **10.1002/cmdc.201300271**

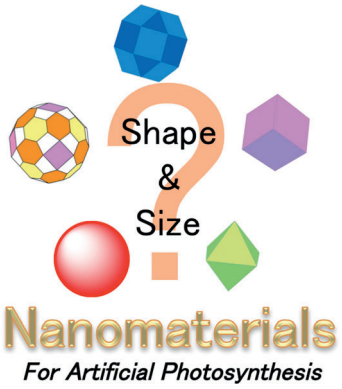
Computational Drug Design

K. L. Whalen, A. C. Chau, M. A. Spies*

In silico Optimization of a Fragment-Based Hit Yields Biologically Active, High-Efficiency Inhibitors for Glutamate Racemase

FERM conclusions: A novel lead compound for inhibition of the antibacterial drug target, glutamate racemase, was optimized for both potency and lipophilic efficiency. A hybrid MD–docking and scoring scheme, FERM-SMD, was used to predict the relative potencies of potential derivatives prior to chemical synthesis.





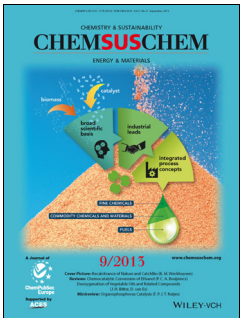
ChemSusChem
DOI: **10.1002/cssc.201300361**

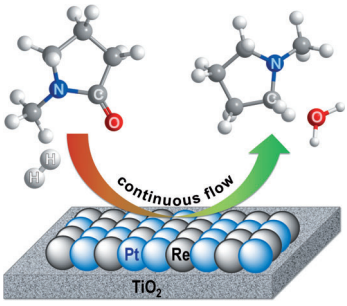
Arificial Photosynthesis

S. Fukuzumi,* Y. Yamada

Shape- and Size-Controlled Nanomaterials for Artificial Photosynthesis

Taking control: The focus is on the control of shape and size of nanomaterials utilized in the development of light-harvesting and charge-separation nanomaterials as well as nanosized catalysts for water oxidation and reduction in artificial photosynthesis. The efficiency of metal and metal-oxide nanoparticle catalysts can be improved by controlling the shapes and sizes of the nanoparticles. Shape- and size-controlled nanoparticles aimed to be utilized in artificial photosynthesis are reviewed.





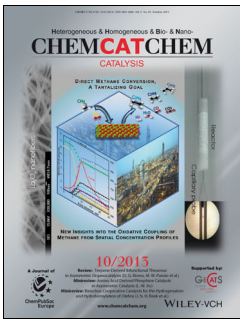
ChemCatChem
DOI: **10.1002/cctc.201300431**

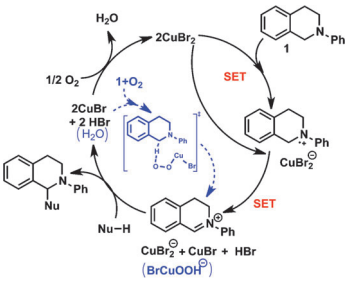
Catalysis in Flow

J. Coetzee, H. G. Manyar, C. Hardacre, D. J. Cole-Hamilton*

The First Continuous Flow Hydrogenation of Amides to Amines

Hydrogen goes with the flow: Conversion of amides into amines is usually achieved with stoichiometric amounts of metal hydrides, which generate large amounts of waste. Catalytic hydrogenation represents an environmentally benign alternative for this conversion, whereas flow catalysis allows catalyst separation and high throughput. Here, we combine amide hydrogenation and flow catalysis for the first time.





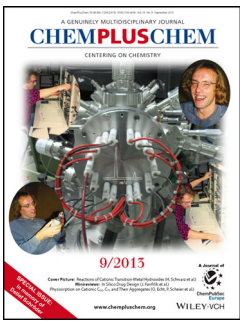
ChemPlusChem
DOI: **10.1002/cplu.201300117**

Reaction Mechanisms

G.-J. Cheng, L.-J. Song, Y.-F. Yang, X. Zhang,* O. Wiest,* Y.-D. Wu*

Computational Studies on the Mechanism of the Copper-Catalyzed sp^3-C–H Cross-Dehydrogenative Coupling Reaction

SET in stone? A computational study on the mechanism of the copper-catalyzed, aerobic cross-dehydrogenative coupling reaction of tetrahydroisoquinoline has been conducted. The calculations support a single-electron transfer (SET) mechanism, but also reveal an alternative mechanism in which O_2 is directly involved.

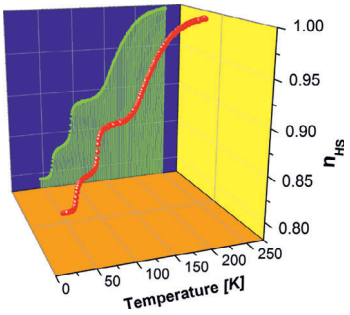


3D Spin-Crossover Nanosystems

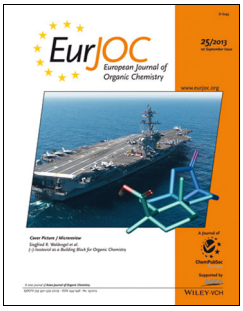
D. Chiruta, J. Linares,* M. Dimian, Y. Alayli, Y. Garcia*

Role of Edge Atoms in the Hysteretic Behaviour of 3D Spin Crossover Nanoparticles Revealed by an Ising-Like Model

The effects of system size, pressure and short-/long-range interactions for incomplete spin transitions, modelled by using a 3D Ising-like model, are discussed.



Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.201300757**

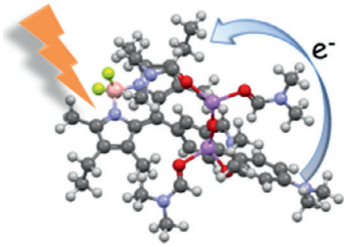


Photophysics

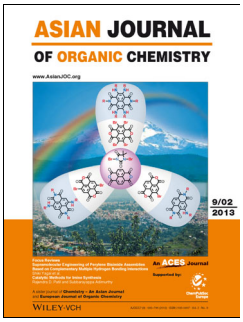
A. C. Benniston,* S. Yang, H. Lemmetyinen, N. V. Tkachenko*

Complexation Enhanced Excited-State Deactivation by Lithium Ion Coordination to a Borondipyrromethene (Bodipy) Donor–Bridge–Acceptor Dyad

A Bodipy-based dyad comprising a donor–bridge–acceptor motif was prepared. Fast electron transfer occurs from the amino donor to the Bodipy acceptor following excitation. The complexation of lithium ions to the 2,2′-biphenol group in the bridge facilitates through-bridge electron transfer.



Eur. J. Org. Chem.
DOI: **10.1002/ejoc.201300867**

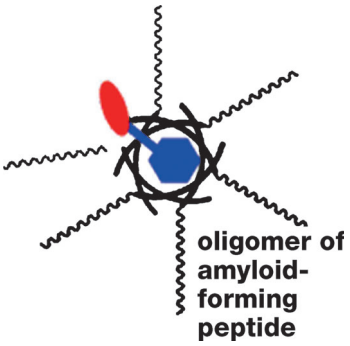


Artificial Proteases

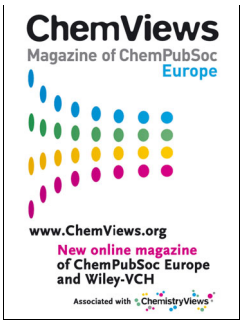
J. Suh*

Progress in Designing Artificial Proteases: A New Therapeutic Option for Amyloid Diseases

Man-made: This Focus Review describes the evolution of artificial proteases. The evolution took place though discovery of catalytic centers for peptide hydrolysis, attachment of substrate-recognition sites to the catalytic centers, and the advent of target-selective artificial proteases. Application of the target-selective artificial proteases led to a therapeutic option for amyloid diseases, such as Alzheimer's disease and diabetes.



Asian J. Org. Chem.
DOI: **10.1002/ajoc.201300135**



Chemical Industry

Chemical Industry Federation of Finland/ChemViews

The chemical sector is very important for the small country of Finland. In recent years it has grown to be Finland's most important export industry, with the value of exports totaling approximately EUR 13.3 billion in 2012. ChemViews magazine gives an overview of this and other trends from Finland's chemical industry.

ChemViews magazine
DOI: **10.1002/chemv.201300094**