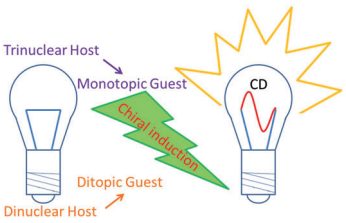
Host-Guest Complexes

M. V. Escárcega-Bobadilla, G. Salassa, M. Martínez Belmonte, E. C. Escudero-Adán, A. W. Kleij*

Versatile Switching in Substrate Topicity: Supramolecular Chirality Induction in Di- and Trinuclear Host Complexes

Host with the most! Supramolecular hosts based on bis-Zn(salphen) scaffolds have been prepared that allow for either monotopic or ditopic binding of suitable chiral guest molecules; this binding results in chirogenesis effects that can be programmed through rigidification of the host by simple cation addition. This new host has potential for the determination of the absolute configurations of various chiral substrates through either di- or monotopic binding modes.



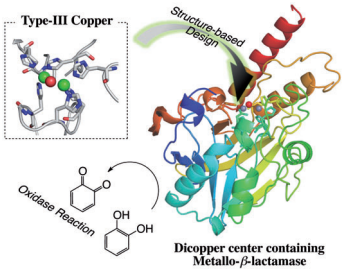
Chem. Eur. J.
DOI: **10.1002/chem.201200335**

Artificial Metalloenzymes

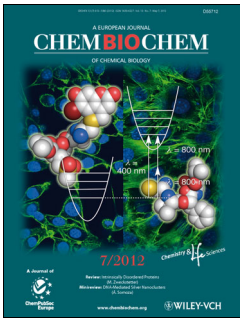
N. Fujieda,* A. Hasegawa, K.-i. Ishihama, S. Itoh*

Artificial Dicopper Oxidase: Rational Reprogramming of Bacterial Metallo-β-lactamase into a Catechol Oxidase

Teaching metalloenzymes new tricks: An artificial type III dicopper oxidase has been developed using a hydrolytic enzyme, metallo-β-lactamase, as a metal-binding platform. The triple mutant D88G/S185H/P224G redesigned by computer-assisted structural analysis showed spectroscopic features similar to those of type III copper proteins and exhibited a high catalytic activity in the oxidation of catechols under aerobic conditions.



Chem. Asian J.
DOI: **10.1002/asia.201101014**

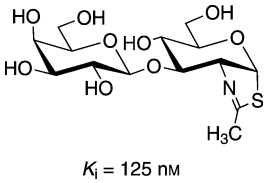


Carbohydrates

M. Hattie, A. W. Debowski, K. A. Stubbs*

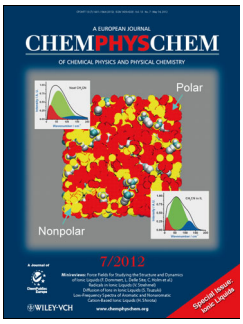
Development of Tools to Study Lacto-*N*-Biosidase: An Important Enzyme Involved in the Breakdown of Human Milk Oligosaccharides

Milk and sugar? The elucidation of the catalytic mechanism and the development of the first known inhibitor for lacto-*N*-biosidases, which are important enzymes involved in the breakdown of human milk oligosaccharides, are described.



K_i = 125 nM

ChemBioChem
DOI: **10.1002/cbic.201200135**

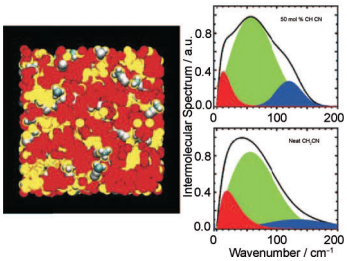


Molecular Dynamics

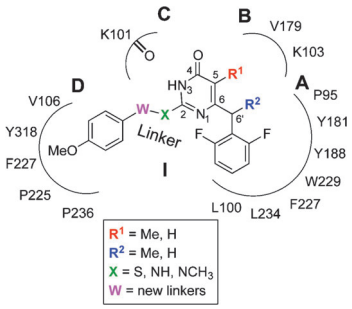
F. Bardak, D. Xiao, L. G. Hines, Jr., P. Son, R. A. Bartsch, E. L. Quitevis,* P. Yang, G. A. Voth*

Nanostructural Organization in Acetonitrile/Ionic Liquid Mixtures: Molecular Dynamics Simulations and Optical Kerr Effect Spectroscopy

Solute–solvent interactions in imidazolium-based ionic liquids are complex. Dipolar solutes, such as CH_3CN, tend to be located at the interfacial region between the charged-order ionic networks (red) and the nonpolar alkyl domains (yellow), with the nitrile groups pointing toward the ionic network, as shown in snapshots obtained from molecular dynamics simulations of CH_3CN/ionic liquid mixtures. Optical Kerr effect spectroscopic measurements suggest that the solute–solvent interactions are governed by strong ion–dipole forces in these mixtures.



ChemPhysChem
DOI: **10.1002/cphc.201200026**



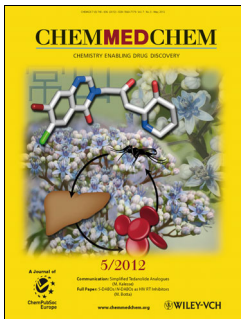
Antiviral Agents

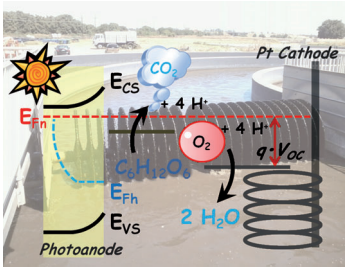
M. Radi, M. Pagano, L. Franchi, D. Castagnolo, S. Schenone, G. Casaluce, C. Zamperini, E. Dreassi, G. Maga, A. Samuele, E. Gonzalo, B. Clotet, J. A. Esté, M. Botta*

Synthesis, Biological Activity, and ADME Properties of Novel *S*-DABOs/*N*-DABOs as HIV Reverse Transcriptase Inhibitors

Keeping a good profile: A new series of *S*-DABO/*N*-DABO derivatives were synthesized to gather additional SAR information on the C2-position and in particular to improve ADME properties while maintaining a good activity profile against HIV-1 RT. The most interesting compounds were experimentally evaluated for their in vitro ADME properties (PAMPA permeation, water solubility, and metabolic stability) to get a reliable indication of their plasma levels after oral administration.

ChemMedChem
DOI: **10.1002/cmdc.201200056**





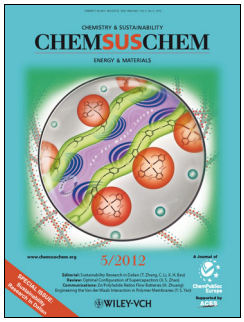
Fuel Cells

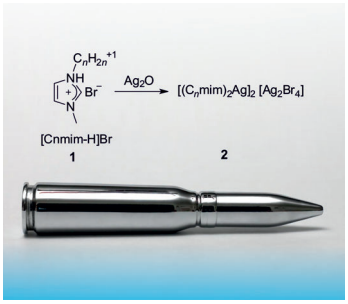
R. L. Chamousis, F. E. Osterloh*

A Light-Assisted Biomass Fuel Cell for Renewable Electricity Generation from Wastewater

Power from waste: Treatment of municipal waste water in the US consumes $25 Billion annually and a significant fraction of US energy. Here, we describe systematic studies on TiO_2/Pt and WO_3/Pt photoelectrochemical cells that can oxidize organic water contaminants with artificial light or with sunlight while generating electricity at the same time.

ChemSusChem
DOI: **10.1002/cssc.201200016**





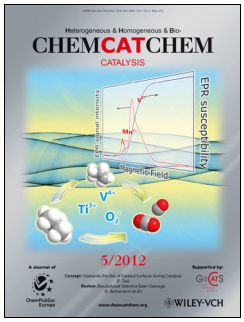
CO_2 Fixation

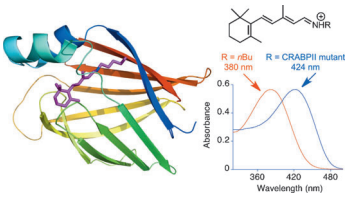
Z. Taşcı, A. Kunduracıoğlu, İ. Kani, B. Çetinkaya*

A New Application Area for Ag-NHCs: CO_2 Fixation Catalyst

A silver bullet for CO_2 fixation: The first example of the silver-NHC (NHC: N-heterocyclic carbene) catalyzed cycloaddition of CO_2 to terminal epoxides is reported. The choice of NHC substituents, halides, and the nature of additives were determined to be important. Recycling experiments showed that the catalyst could be used at least seven times without loss of activity and selectivity.

ChemCatChem
DOI: **10.1002/cctc.201100430**





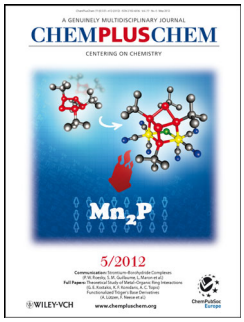
Bioorganic Chemistry

K. S. S. Lee, T. Berbasova, C. Vasileiou, X. Jia, W. Wang, Y. Choi, F. Nossoni, J. H. Geiger,* B. Borhan*

Probing Wavelength Regulation with an Engineered Rhodopsin Mimic and a C15-Retinal Analogue

Shield and control: The application of a protein design strategy to interrogate the perception of color is described. Cellular retinoic acid binding protein II (see structure) was used first to show that complete encapsulation of the chromophore is critical to achieve an opsin shift comparable to the one observed for rod rhodopsin, and second to show that a rhodopsin protein mimic capable of binding a retinoid analogue responds to changes in electrostatic environments.

ChemPlusChem
DOI: **10.1002/cplu.201100082**

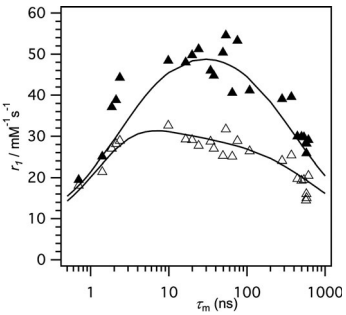


Structure–Relaxivity Relationships

P. Caravan,* Z. Zhang

Structure–Relaxivity Relationships among Targeted MR Contrast Agents

The effect of changing a single donor atom in a gadolinium(III) complex targeting human serum albumin can be seen in the graphic. The single donor group modification alters inner-sphere water exchange by three orders of magnitude and changes relaxivity by a factor of five. Water exchange can be rationally tuned to optimize relaxivity.



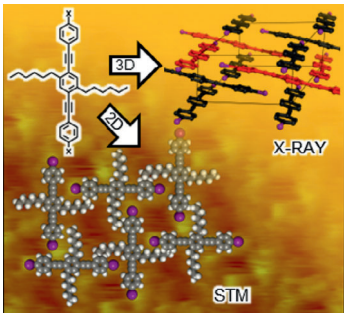
Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.201101364**

Intermolecular Interactions

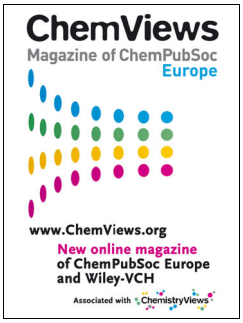
N. M. Jenny, H. Wang, M. Neuburger, H. Fuchs, L. Chi,* M. Mayor*

Synthesis and Solid-State Investigations of Oligo-Phenylene–Ethynylene Structures with Halide End-Groups

We have synthesized a series of halogen-end-capped oligo-phenylene-ethynylenes to study interactions at the solid/liquid interface and in crystal structures. Here we probe the interplay and diversity of intermolecular interactions between halide end-groups and oligo-phenylene-ethynylene backbones through solution depositions (2D) and X-ray crystal structures (3D). The STM images and crystal structures reveal a striking complementarity in each case.



Eur. J. Org. Chem.
DOI: **10.1002/ejoc.201200033**



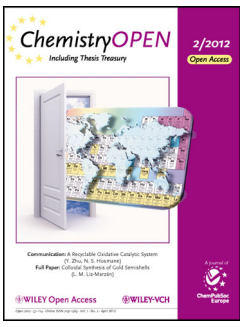
Biocides Regulation

Vera Koester

New Biocides Legislation – Interview with Jukka Malm

All active substances that are put into biocidal products marketed in Europe have to be approved by the Biocides Directive. The Directive has been updated recently with the changes coming into effect this summer. Jukka Malm, Director Regulatory Affairs, European Chemicals Agency, discusses the changes to the regulation.

ChemViews magazine
DOI: **10.1002/chemv.201200033**

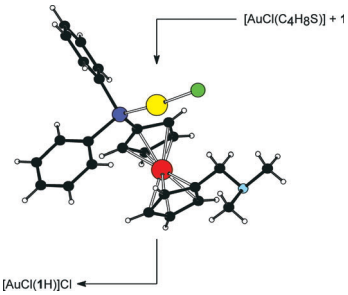


Ferrocene Ligands

P. Štěpnička,* M. Zábranský, I. Císařová

An Alternative Preparation of 1-(*N*,*N*-Dimethylaminomethyl)-1′-(diphenylphosphanyl)ferrocene: Synthesis and Structural Characterization of Au^{I} and Pd^{II} Complexes with this Hybrid Ligand

Simple ligands behave complex! 1-(*N*,*N*-Dimethylaminomethyl)-1′-(diphenylphosphanyl)ferrocene (**1**) was prepared from 1,1′-dibromoferrocene and used as a donor for Au^{I} and Pd^{II} ions. Compound **1** coordinates Au^{I} as a simple phosphane, and its free amine is easily protonated. A similar observation was made with Pd^{II}, for which a ligand-bridged dimer $[(\mu\text{-}\mathbf{1})PdCl_2]_2$ was also isolated.



ChemistryOpen
DOI: **10.1002/open.201200004**