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Iridium

H. Junge, N. Marquet, A. Kammer, S. Denurra, M. Bauer,* S. Wohlrab, F. Gärtner, M.-M. Pohl, A. Spannenberg, S. Gladiali, M. Beller*

Water Oxidation with Molecularly Defined Iridium Complexes: Insights into Homogeneous Versus Heterogeneous Catalysis

Ir walks a fine line: Molecularly defined Ir complexes and IrO_2 nanoparticles have been applied in the water oxidation reaction with cerium ammonium nitrate (CAN) as oxidant and compared (see scheme). The conversion of the first to the latter has been investigated by means of XANES, EXAFS, and STEM.



Chem. Eur. J.

DOI: 10.1002/chem.201201472

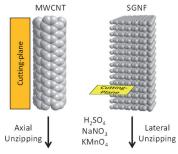


Graphene

C. K. Chua, Z. Sofer, M. Pumera*

Graphene Sheet Orientation of Parent Material Exhibits Dramatic Influence on Graphene Properties

Stacked actors: Electrochemical analysis indicated that pristine stacked graphene nanofibers (PSGNs) gave at least a twofold-higher HET rate than its thermally reduced product and graphene that was obtained from unzipped carbon nanotubes (MWCNTs).



Chem. Asian J.

DOI: 10.1002/asia.201200409

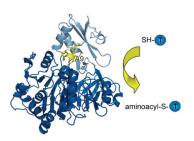


Nonribosomal Peptide Synthetases

V. Bučević-Popović,* M. Šprung, B. Soldo, M. Pavela-Vrančič*

The A9 Core Sequence from NRPS Adenylation Domain Is Relevant for Thioester Formation

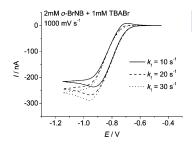
Finding the right partner: The role of the A9 core sequence in the NRPS adenylation domain has been investigated by mutational analysis. The A9 region plays a role in the second reaction step, in which it might serve to properly position residues important for the interaction with a partner T-domain, and/or stabilising the thioester-forming conformation of the enzyme.



ChemBioChem

DOI: 10.1002/cbic.201200309





Chem Phys Chem DOI: 10.1002/cphc.201200480

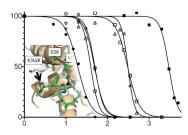
Electrochemistry

Y. Wang, E. O. Barnes, R. G. Compton*

New Chemical Insights Using Weakly Supported Voltammetry: The Reductive Cleavage of Aryl-Br Bonds is Reversible

Cyclic voltammetry carried out at a wide range of supporting electrolyte concentrations and compositions can elucidate additional kinetic and mechanistic details of the electrochemical reduction of aryl halides (see picture). The cleavage of the C-Br bond is reversible, driven by H abstraction and the second electron transfer. This is a new chemical insight, as the cleavage of such bonds has usually been regarded as irreversible.





ChemMedChem

DOI: 10.1002/cmdc.201200286

Antitumor Agents

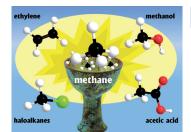
C1 Chemistry

R. A. Entwistle, R. S. Rizk, D. M. Cheng, G. H. Lushington, R. H. Himes, M. L. Gupta, Jr.*

Differentiating between Models of Epothilone Binding to Microtubules Using Tubulin Mutagenesis, Cytotoxicity, and Molecular Modeling

Stabilizing microtubules with small molecules is a proven strategy for cancer treatment. Site-directed mutagenesis of five sites in the epothilone binding pocket of tubulin created a panel of yeast strains with graded sensitivity to epothilone B. In vivo cytotoxicity data were combined with molecular mechanics simulations to discriminate between proposed models of epothilone binding to microtubules.





ChemSusChem

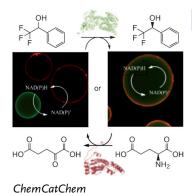
DOI: 10.1002/cssc.201200299

C. Hammond, S. Conrad, I. Hermans*

Oxidative Methane Upgrading

What a challenge! The oxidative coupling and partial oxidation of methane by economically feasible methods remain among the holy grails of chemistry. This Minireview highlights important developments and summarises the pertaining challenges that need to be tack-





DOI: 10.1002/cctc.201200146

Supported Enzyme Cascades

J. Rocha-Martín, B. d. l. Rivas, R. Muñoz, J. M. Guisán,* F. López-Gallego*

Rational Co-Immobilization of Bi-Enzyme Cascades on Porous Supports and their Applications in Bio-Redox Reactions with In Situ Recycling of Soluble Cofactors

Better together: Co-immobilization was used to assemble three bioredox orthogonal cascades with in situ cofactor-regeneration. These procedures were more efficient than if the dehydrogenases were immobilized on different carriers.



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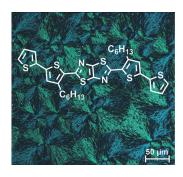


Organic Field-Effect Transistors

S. Van Mierloo, K. Vasseur, N. Van den Brande, A. E. Boyukbayram, B. Ruttens, S. D. Rodriguez, E. Botek, V. Liégeois, J. D'Haen, P. J. Adriaensens, P. Heremans, B. Champagne, G. Van Assche, L. Lutsen, D. J. Vanderzande,* W. Maes*

Functionalized Dithienylthiazolo[5,4-d]thiazoles For Solution-Processable Organic Field-Effect Transistors

On the move: A series of dithienylthiazolo [5,4-d]thiazole (DTTzTz) semiconductors has been synthesized and investigated as active materials in solution-processed organic field-effect transistors. Spin-coated films of one of the derivatives showed a micrometer scale fibrillar texture and high field-effect mobilities ($10^{-3} \, \text{cm}^2 \, \text{V}^{-1} \, \text{s}^{-1}$) were observed. This molecule represents the first example of a highly soluble DTTzTz-based small organic compound for which a reasonable FET behavior was observed.



Chem Plus Chem

DOI: 10.1002/cplu.201200132

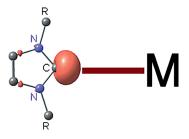


N-Heterocyclic Carbenes

A. Kumar, P. Ghosh*

Studies of the Electronic Properties of N-Heterocyclic Carbene Ligands in the Context of Homogeneous Catalysis and Bioorganometallic Chemistry

Towards understanding the key attributes that define the influence of N-heterocyclic carbenes on catalysis, our efforts, involving combined experimental and computational approaches, in looking into a variety of catalytic and biomedical applications of these compounds are summarized.



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201200622

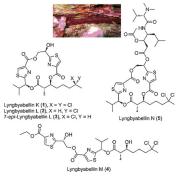


Cytotoxic Lipopeptides

H. Choi, E. Mevers, T. Byrum, F. A. Valeriote, W. H. Gerwick*

Lyngbyabellins K-N from Two Palmyra Atoll Collections of the Marine Cyanobacterium *Moorea bouillonii*

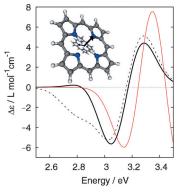
Two independent collections of the marine cyanobacterium *Moorea bouillonii* led to the isolation of five lipopeptides of the lyngbyabellin structure class. Their structures were elucidated by various spectroscopy, synthesis, and chromatography techniques. Lyngbyabellin N showed strong cytotoxic activity against the HCT116 colon cancer cell line (IC $_{50}=40.9\pm3.3$ nm).



Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201200691





ChemistryOpen

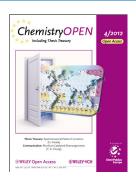
DOI: 10.1002/open.201200020

Computational Chemistry

B. Moore, II, J. Autschbach*

Density Functional Study of Tetraphenylporphyrin Long-Range Exciton Coupling

Tune it! Time dependent density functional theory (TDDFT) calculations were performed to study the exciton coupling circular dichroism (CD) of tetraphenylporphyrin (TPP). Calculated TDDFT data were used as input for a 'matrix-method' dipole coupling model. A TPP dimer model was set up to reproduce the exciton CD of a brevetoxin derivative with TPP substituents at a spatial separation of >40~Å.





ChemViews magazine
DOI: 10.1002/chemv.201200105

Reactivity and Bonding

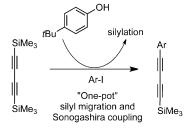
Synthetic Methods

V. Köster

Sason Shaik on the Motivation Behind his Research

Professor Sason Shaik, The Hebrew University, Jerusalem, Israel, talks about the motivation behind his research and how that has led him into diverse areas such as new theoretical models for bonding and enzymatic activation.





Asian J. Org. Chem.

DOI: 10.1002/ajoc.201200018

M. Shigeta,* J. Watanabe, G.-i. Konishi*

Preparation of Arylbutadiyne Derivatives by Silyl Migration Inspired by the Mukaiyama Protocol

One at a time: A one-pot monodesilylation and arylation of a silyl end-capped butadiyne is presented. Inspired by the Mukaiyama aldehyde alkynylation protocol, this method furnishes arylbutadiynes, which are potentially useful synthetic intermediates in the synthesis of other complex or linear structures. The transformation is achieved with reagents that are easily handled and avoids the need to isolate highly volatile intermediates.

