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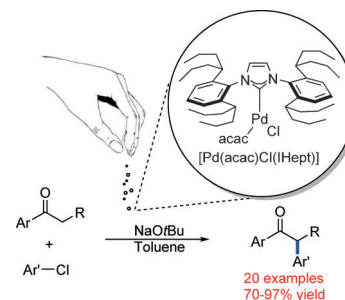


Organic Chemistry

E. Marelli, M. Corpet, S. R. Davies, S. P. Nolan*

Palladium-Catalyzed α -Arylation of Arylketones at Low Catalyst Loadings

Less than a pinch: Arylation of ketones at very low catalyst loadings has been achieved by using a member of the Pd-ITent-based pre-catalyst family. The system has a wide substrate scope, including functionalized partners, and gives the desired product in good to excellent yields. The synthesis of a key pharmaceutical intermediate was also achieved using this protocol (see scheme; acac = acetylacetonate; ITent = Tentacular Imidazo-2-ylidene; IHept = 1,3-bis(2,6-di(heptan-4-yl)phenyl)imidazo-2-ylidene).



Chem. Eur. J.
DOI: 10.1002/chem.201404900

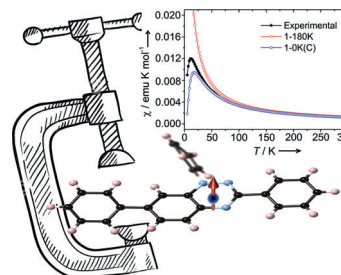


Computational Chemistry

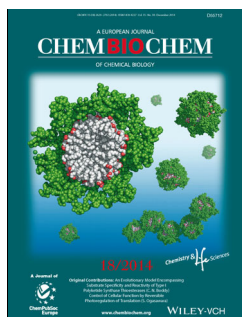
M. Fumanal, S. Vela,* J. Ribas-Ariño, J. J. Novoa

On the Importance of Thermal Effects and Crystalline Disorder in the Magnetism of Benzotriazinyl-Derived Organic Radicals

Making sense of disorder: The first complete computational study on the magnetic properties of two benzotriazinyl-derived radicals is reported (see picture). The thermal contraction of the crystal and crystalline disorder are elements to be reckoned with for the rational design of future materials of this family of compounds.



Chem. Asian J.
DOI: 10.1002/asia.201402871

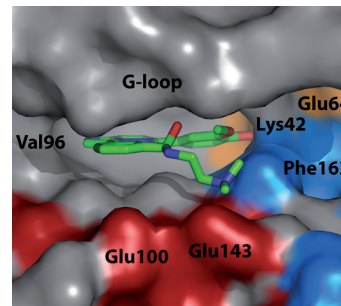


Enzyme Inhibitors

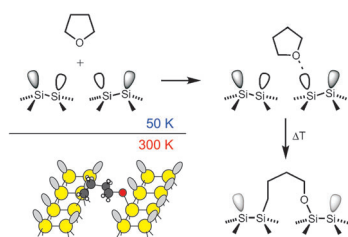
T. S. Wilbek, T. Skovgaard, F. J. Sorrell, S. Knapp, J. Berthelsen, K. Strømgaard*

Identification and Characterization of a Small-Molecule Inhibitor of Death-Associated Protein Kinase 1

A novel imidazo-pyrimidine inhibitor of DAPK1 that undergoes class-specific interactions and extends into the substrate recognition site has been identified. This inhibitor is a good starting point for the development of selective and potent inhibitors of DAPK1, with potential use against stroke and ischemia.



ChemBioChem
DOI: 10.1002/cbic.201402512



ChemPhysChem

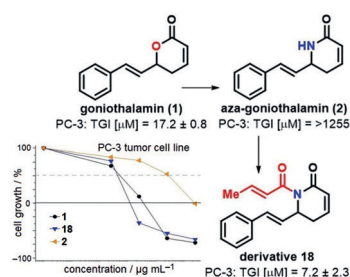
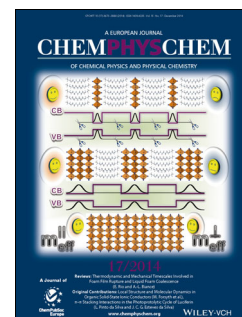
DOI: 10.1002/cphc.201402486

Surface Chemistry

G. Mette, M. Reutzel, R. Bartholomäus, S. Laref, R. Tonner, M. Dürr,* U. Koert, U. Höfer

Complex Surface Chemistry of an Otherwise Inert Solvent Molecule: Tetrahydrofuran on Si(001)

The road less taken: The reaction mechanism of tetrahydrofuran (THF) on Si(001) was investigated using scanning tunneling microscopy and photoelectron spectroscopy at variable temperatures. At low temperature, a datively bound intermediate of THF on Si(001) was isolated. Heating the surface to room temperature leads to ether cleavage resulting in a configuration which bridges two dimer rows of the Si(001) surface.



ChemMedChem

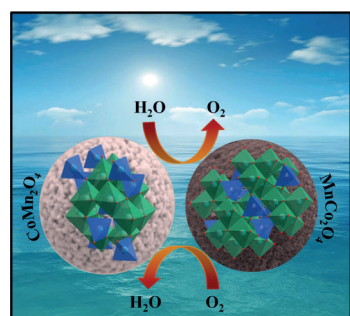
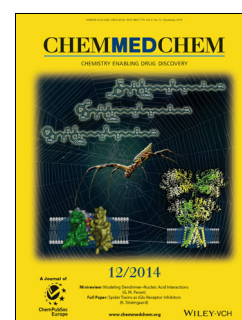
DOI: 10.1002/cmdc.201402292

Antitumor Agents

R. C. Barcelos, J. C. Pastre, D. B. Vendramini-Costa, V. Caixeta, G. B. Longato, P. A. Monteiro, J. E. de Carvalho, R. A. Pilli*

Design and Synthesis of N-Acylated Aza-Goniiothalamine Derivatives and Evaluation of Their in Vitro and in Vivo Antitumor Activity

In vivo l'importance! We conducted antiproliferation assays of a library of aza derivatives of goniiothalamine (**1**) against a panel of tumor cell lines. The most potent compound, **18**, led to reactive oxygen species generation, apoptosis, and G₂/M cell-cycle arrest in prostate PC-3 cells, but it failed to inhibit tumor growth. Surprisingly, aza-goniiothalamine (**2**), which was shown to be much less toxic in vitro, inhibited Ehrlich tumor development in mice.



ChemSusChem

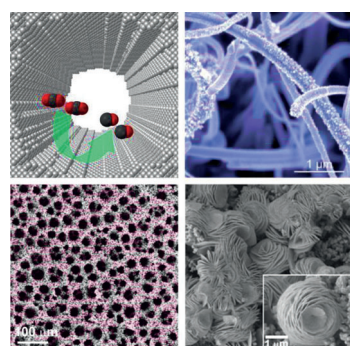
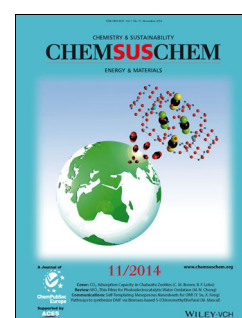
DOI: 10.1002/cssc.201402699

Water Oxidation

P. W. Menezes, A. Indra, N. R. Sahraie, A. Bergmann, P. Strasser,* M. Driess*

Cobalt–Manganese-Based Spinel as Multifunctional Materials that Unify Catalytic Water Oxidation and Oxygen Reduction Reactions

All-in-one: Porous cobalt-manganese-based spinels are prepared from their respective carbonate precursors and are used as highly effective multifunctional catalysts for the unification of electrochemical, oxidant-driven, and photochemical oxygen evolution as well as the oxygen reduction reaction.



ChemCatChem

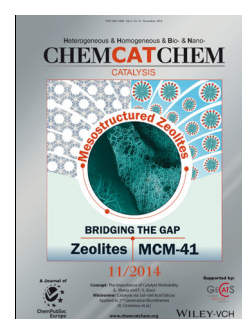
DOI: 10.1002/cctc.201402669

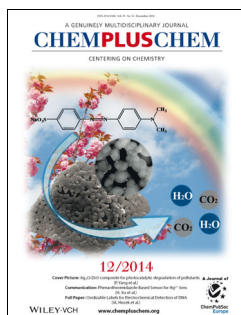
Carbon Dioxide Reduction

Q. Lu, J. Rosen, F. Jiao*

Nanostructured Metallic Electrocatalysts for Carbon Dioxide Reduction

Small is beautiful: Electrochemical CO₂ reduction is an attractive approach to convert CO₂ produced in power plants, refineries, and petrochemical plants to liquid fuels or useful chemicals. Recent progress in nanostructured metallic catalysts has exhibited tremendous promise for such realization. This review takes a closer look at those studies, and future research directions are proposed and discussed.



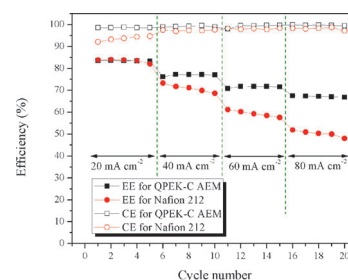


Redox Flow Batteries

S. Yun, J. Parrondo, V. Ramani*

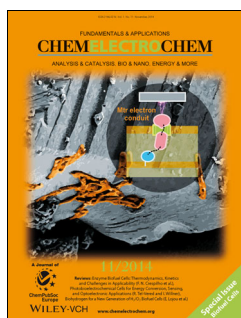
A Vanadium–Cerium Redox Flow Battery with an Anion-Exchange Membrane Separator

Membranes in charge: Quaternized cardo-poly(etherketone) (QPEK-C) anion-exchange membranes (AEMs) have been prepared and employed as a separator in a redox flow battery [carbon felt | V^{3+} , V^{2+} (0.5 M) || carbon felt | Ce^{4+} , Ce^{3+} (0.5 M)]. The low cation permeability of the AEM together with its good mechanical and chemical stability give this material improved coulombic efficiency (CE) and energy efficiency (EE) during cycling (see figure).



ChemPlusChem

DOI: 10.1002/cplu.201402096

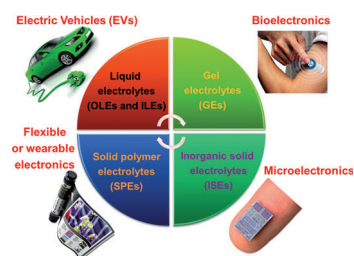


Energy Storage

Y. Wang, W.-H. Zhong*

Development of Electrolytes towards Achieving Safe and High-Performance Energy-Storage Devices: A Review

Liquid, solid, or gel? High-performance electrolytes are important for the success of advanced energy-storage devices. From the view of battery structures and the electrolyte, this Review not only summarizes and discusses the up-to-date development of various electrolyte materials (liquids, solids, and gels), but also emphasizes a comprehensive understanding of electrolyte properties, which is critical for the design of high-performance electrolytes.



ChemElectroChem

DOI: 10.1002/celec.201402277

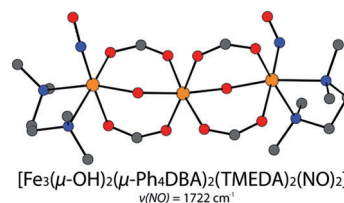


Nitrosylated Iron Complexes

E. Victor, M. A. Minier, S. J. Lippard*

Synthesis and Characterization of a Linear Dinitrosyl-Triiron Complex

The complex $[Fe_3(\mu-OH)_2(\mu-Ph_4DBA)_2(TMEDA)_2(NO)_2](OTf)$ was synthesized and spectroscopically characterized. Its properties resemble those of a proposed intermediate observed during the catalytic reduction of nitric oxide by flavodiiron reductases.



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201402543

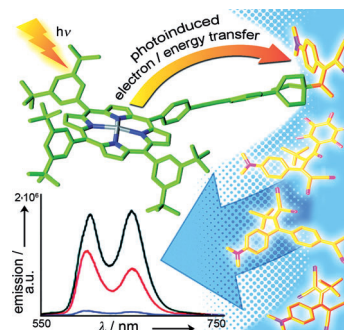


Donor–Acceptor Systems

L. M. Urner, M. Sekita, N. Trapp, W. B. Schweizer, M. Wörle, J.-P. Gisselbrecht, C. Boudon, D. M. Guldi,* F. Diederich*

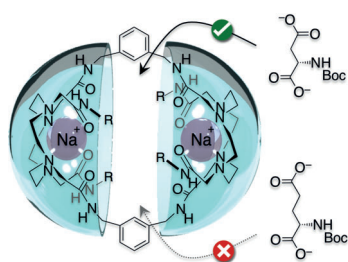
Systematic Variation of Cyanobuta-1,3-dienes and Expanded Tetracyanoquinodimethane Analogues as Electron Acceptors in Photoactive, Rigid Porphyrin Conjugates

The modular synthesis and characterization of a series of rigid Zn^{II} porphyrin conjugates is described. The push–pull chromophores incorporated as electron acceptors feature first reduction potentials ranging from -1.78 to -0.58 V vs. Fe^+/Fc , and affect the extent of Zn^{II} porphyrin fluorescence quenching according to their acceptor strength.



Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201403252



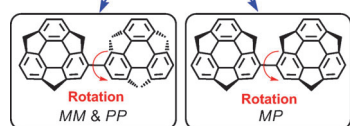
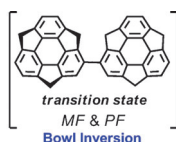
ChemistryOpen
DOI: 10.1002/open.201402049

Molecular Sensors

H. Ito,* S. Shinoda

Chirality Sensing and Size Discrimination of Anions by Macrocyclic Cyclen–Disodium Complexes

Chirality on Na⁺: The first example of chirality sensing on Na⁺ was achieved by a macrocyclic host composed of two octadentate cyclen–Na⁺ complexes. Chiral *N*-Boc-Asp dianions coordinated to the Na⁺ at the cavity, resulting in the chirality induction of the cage molecule, but *N*-Boc-Glu dianion, which is one carbon longer, did not.



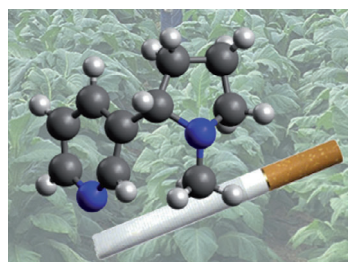
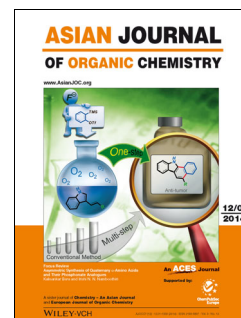
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201402226

Polyaromatic Hydrocarbons

B. B. Shrestha, S. Karanjit, S. Higashibayashi,* T. Amaya, T. Hirao,* H. Sakurai

Investigation of the Dynamic Behavior of Bisumanenyl

Flippin' bowls: The conformational dynamic behavior of bisumanenyl was fully elucidated by a combination of ¹H NMR experiments and DFT calculations.



ChemViews magazine
DOI: 10.1002/chemv.201400107

Natural Products

S. Streller, K. Roth

The Chemistry of Tobacco

Worldwide, roughly 15 tons of nicotine from tobacco makes its way daily into smokers' lungs. That alone is sufficient reason to consider this particular natural product more closely. In this part of its article series on tobacco, *ChemViews Magazine* looks at the chemical changes between the harvest and a finished cigarette.

