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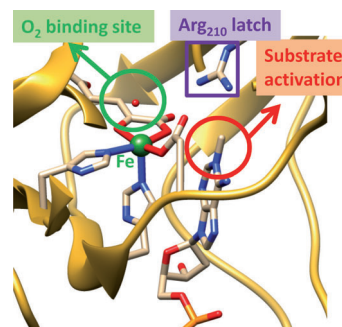


DNA Damage

M. G. Quesne, R. Latifi, L. E. Gonzalez-Ovalle, D. Kumar, S. P. de Visser*

Quantum Mechanics/Molecular Mechanics Study on the Oxygen Binding and Substrate Hydroxylation Step in AlkB Repair Enzymes

Right of passage: A combination of density functional theory and quantum mechanics/molecular mechanics studies is presented on the oxygen activation by AlkB repair enzymes. These studies identify the substrate and oxygen binding sites and the origin of their structural separation. It is also shown that the Arg₂₁₀ residue in the active site acts as a latch that only allows the iron(IV)-oxo to pass and react with substrate (see figure).



Chem. Eur. J.
DOI: 10.1002/chem.201303282

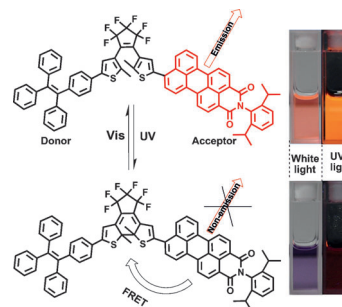


Photochromism

C. Li, H. Yan, G.-F. Zhang, W.-L. Gong, T. Chen, R. Hu, M. P. Aldred,* M.-Q. Zhu*

Photocontrolled Intramolecular Charge/Energy Transfer and Fluorescence Switching of Tetraphenylethene-Dithienylethene-Perylenemonoimide Triad with Donor–Bridge–Acceptor Structure

The matrix reloaded: We report the synthesis and photophysical characterization of a donor–photochromic bridge–acceptor tetraphenylethene-dithienylethene-perylenemonoimide (TPE-DTE-PMI) triad that simultaneously exhibits photocontrolled intramolecular charge/energy transfer and enhanced reversible fluorescence switching, depending on the surrounding matrices.



Chem. Asian J.
DOI: 10.1002/asia.201301071

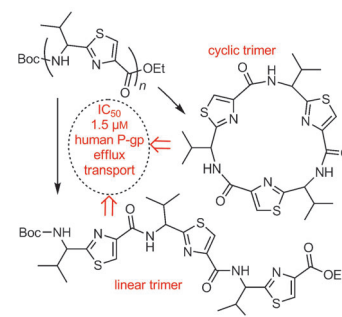


Multidrug Resistance

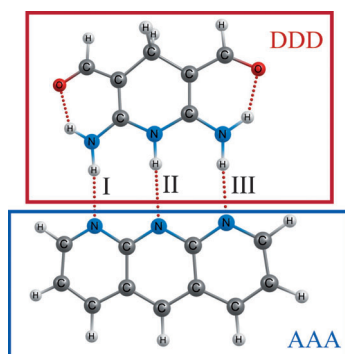
S. Singh, N. R. Prasad, K. Kapoor, E. E. Chufan, B. A. Patel, S. V. Ambudkar,* T. T. Talele*

Design, Synthesis, and Biological Evaluation of (S)-Valine Thiazole-Derived Cyclic and Noncyclic Peptidomimetic Oligomers as Modulators of Human P-Glycoprotein (ABCB1)

Circles and lines: Synthesis of isosteric analogues of QZ59Se-SSS to inhibit the efflux activity of human P-glycoprotein (P-gp) resulted in cyclic trimer and linear trimer compounds as the most potent in the series. These compounds can be further optimized by replacing the thiazole unit with privileged fragments.



ChemBioChem
DOI: 10.1002/cbic.201300565



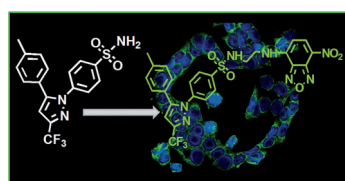
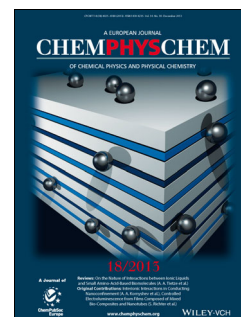
ChemPhysChem
DOI: 10.1002/cphc.201300639

Hydrogen Bonds

A. H. D. Lopez,* G. F. Caramori,* D. F. Coimbra, R. L. T. Parreira, É. H. da Silva

The Two Faces of Hydrogen-Bond Strength on Triple AAA–DDD Arrays

Three in a row: Systems connected through multiple hydrogen bonds are the cornerstone of molecular recognition processes in biology, and are increasingly being employed in molecular self-assembly processes. The applicability of this phenomenon in the design of new materials is investigated and the effects caused by the presence of substituents in the intermolecular hydrogen bonds quantified in order to contribute to the advancement of this branch of science.



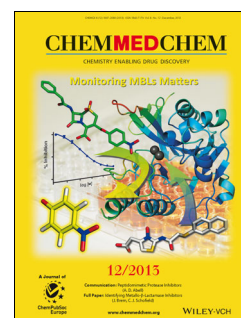
ChemMedChem
DOI: 10.1002/cmdc.201300355

Cancer Imaging

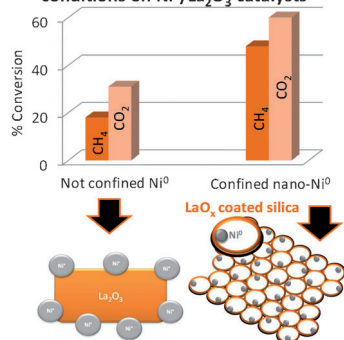
A. Bhardwaj, J. Kaur, F. Wuest,* E. E. Knaus*

Fluorophore-Labeled Cyclooxygenase-2 Inhibitors for the Imaging of Cyclooxygenase-2 Overexpression in Cancer: Synthesis and Biological Studies

Targeted imaging: The association between cyclooxygenase-2 (COX-2) isozyme overexpression and the development of several kinds of human cancer make COX-2 an attractive target for the design of new cancer biomarkers. Herein we describe the synthesis and biological evaluation of a group of fluorescent COX-2 inhibitors for imaging cancer cells that overexpress COX-2.



Dry Reforming of methane under severe conditions on Ni⁰/La₂O₃ catalysts



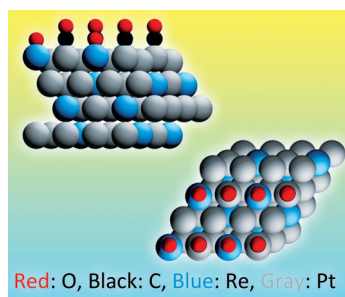
ChemSusChem
DOI: 10.1002/cssc.201300718

Methane Reforming

J.-P. Dacquin, D. Sellam, C. Batiot-Dupeyrat, A. Tougeri, D. Duprez, S. Royer*

Efficient and Robust Reforming Catalyst in Severe Reaction Conditions by Nanoprecursor Reduction in Confined Space

A reformed character: The preparation of highly dispersed nickel-containing oxide material allows the design of a highly active and stable nickel reforming catalyst. Control over the size and size distribution of metallic nanoparticles results in improved catalytic activity in the methane dry reforming reaction. These composite materials also exhibit excellent stability under severe reaction conditions.



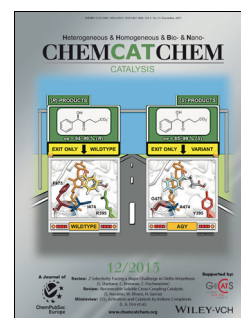
ChemCatChem
DOI: 10.1002/cctc.201300365

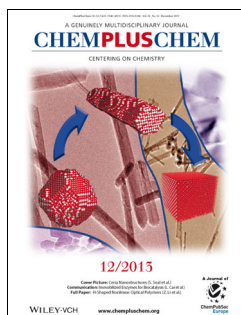
Water Gas Shift

R. Carrasquillo-Flores, J. M. R. Gallo, K. Hahn, J. A. Dumesic, M. Mavrikakis*

Density Functional Theory and Reaction Kinetics Studies of the Water–Gas Shift Reaction on Pt–Re Catalysts

ReOx decorations in a Pt surface: Pt–Re alloys show high activity for low-temperature water–gas shift reactions. Pt atoms serve as the adsorption site for CO molecules, whereas the Re atoms are determined to be in an oxidized state; they act as a promoter for the reaction, by destabilizing the CO molecules.



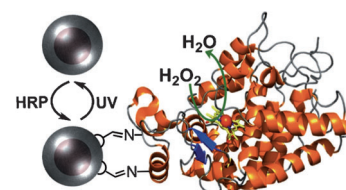


Biocatalysis

L. Cai,* L. Chen, L. Zhang, G. Lu, X. He, S. Zhang, H. Sun, Z. Liu, B. Zhao*

Recyclable, Biocompatible, Magnetic Titanium Dioxide Nanoparticles with Immobilized Enzymes for Biocatalysis

Clean break: Magnetic nanoparticles are fabricated with mesoporous anatase shells, which are biocompatible for enzyme immobilization (see picture; HRP=horseradish peroxidase). The nanobiocatalyst can be easily collected with an external magnet and recycled. Immobilized enzymes with low activity after several cycles can be decomposed with UV radiation and thus the nanoparticles are recyclable for new enzyme immobilization.



ChemPlusChem
DOI: 10.1002/cplu.201300241

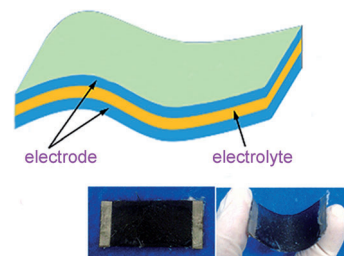


Capacitors

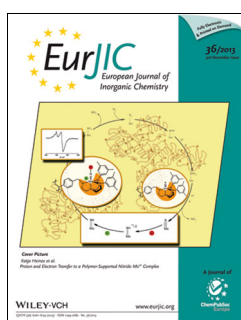
Q. Wang, J. Xu, X. Wang, B. Liu, X. Hou, G. Yu, P. Wang, D. Chen,* G. Shen*

Core-Shell CuCo₂O₄@MnO₂ Nanowires on Carbon Fabrics as High-Performance Materials for Flexible, All-Solid-State, Electrochemical Capacitors

Bend and twist: Flexible supercapacitors are fabricated from electrodes consisting of core-shell CuCo₂O₄@MnO₂ nanowire heterostructures on carbon fabric (see picture), which are prepared by using a simple hydrothermal method. They exhibit high area-specific capacitance, excellent rate capability, and long-term cycling life, even in the bent state.



ChemElectroChem
DOI: 10.1002/celc.201300084

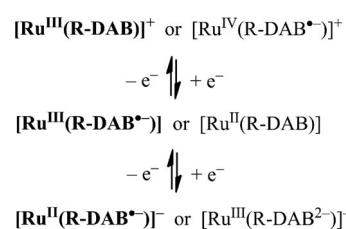


Oxidation States

A. Grupp, M. Bubrin, F. Ehret, Q. Zeng, F. Hartl, H. Kvapilová, S. Zális, W. Kaim*

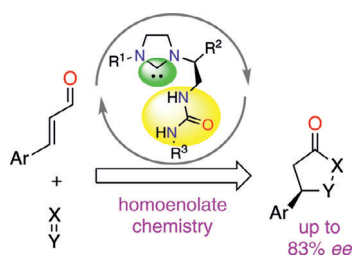
Ru^{II}(α-diimine) or Ru^{III}(α-diimine[−])? Structural, Spectroscopic, and Theoretical Evidence for the Stabilization of a Prominent Metal-to-Ligand Charge-Transfer Excited-State Configuration in the Ground State

[Ru(R-DAB)(acac)₂] (acac = 2,4-pentanedionate, R-DAB = substituted 1,4-diaza-1,3-butadiene) can be described as Ru^{III}(R-DAB[−]) species on the basis of their structures and the absence of solvatochromism. Oxidation yields Ru^{III} complexes, whereas reduction at rather negative potentials requires acceptor substituents and low temperatures in order to be reversible; this indicates that there is substantial charge on the R-DAB ligand.



(dominant alternatives printed in boldface)

Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201301206



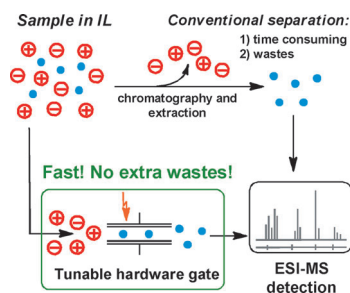
Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201301366

NHC Organocatalysis

F. Nawaz, M. Zaghouni, D. Bonne, O. Chuzel, J. Rodriguez,*
Y. Coquerel*

Design, Synthesis, and Organocatalytic Activity of N-Heterocyclic Carbenes Functionalized with Hydrogen-Bond Donors in Enantioselective Reactions of Homo-enolates

Chiral 1,3-imidazolin-2-ylidene NHCs functionalized with urea-type hydrogen-bond donors have been evaluated as organocatalysts in enantioselective reactions of homo-enolates. Some unprecedented levels of enantioselectivity have been obtained.



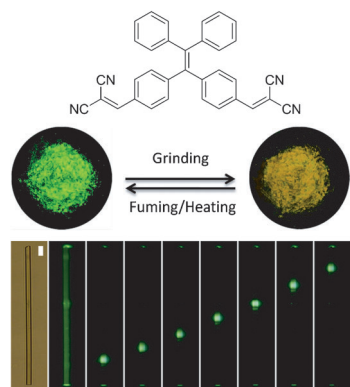
ChemistryOpen
DOI: 10.1002/open.201300022

Analytical Chemistry

L. L. Khemchyan, E. A. Khokhlova, M. M. Seitkalieva, V. P. Ananikov*

Efficient Sustainable Tool for Monitoring Chemical Reactions and Structure Determination in Ionic Liquids by ESI-MS

Simple and effective: A facile procedure for monitoring chemical reactions and characterizing compounds dissolved in ionic liquids is described using the MS/MS technique. Separation of species of interest was carried out using internal electronic gate available in electrospray mass spectrometers, instead of chromatography and extraction. The separation was carried out as a fast (milliseconds) and sustainable (no extra solvents) procedure.



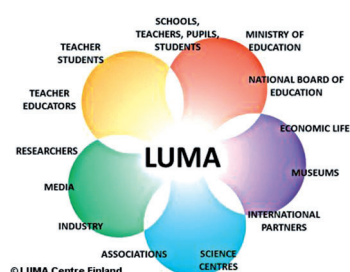
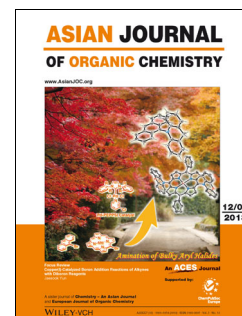
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201300223

Mechanochromism

N. Zhao, C. Zhang, J. W. Y. Lam, Y. S. Zhao, B. Z. Tang*

An Aggregation-Induced Emission Luminogen with Efficient Luminescent Mechanochromism and Optical Waveguiding Properties

Guiding light: A yellow aggregation-induced emission luminogen (TPE-DCV) was synthesized by decorating a tetraphenylethene group with two dicyanovinyl units. This compound exhibits reversible luminescent mechanochromism. Two shapes of microcrystal of TPE-DCV display outstanding optical waveguiding behavior.



ChemViews magazine
DOI: 10.1002/chemv.201300127

Education

M. Pollari

Discover the Joy of Science with LUMA Centre Finland

The Science Education Centre LUMA is a unique project that aims to cultivate an interest and enjoyment of science, technology, and mathematics in children and young people. Activities organized by LUMA include science clubs, events, and summer camps, web-based magazines targeted at children and young people, and training courses for science teachers.

