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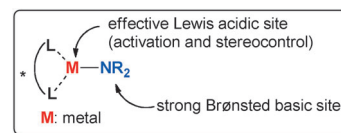


Asymmetric Synthesis

Y. Yamashita, S. Kobayashi*

Metal Amides as the Simplest Acid/Base Catalysts for Stereoselective Carbon–Carbon Bond-Forming Reactions

New possibilities for metal amides as catalysts in highly stereoselective carbon–carbon bond-forming reactions are described (see scheme). Although typical metal amides have been recognized as strong stoichiometric bases for deprotonation of inert or less acidic hydrogen atoms, transition-metal amides, namely silver and copper amides, show interesting abilities and possibilities as one of the simplest acid/base catalysts.



Chem. Eur. J.
DOI: 10.1002/chem.201300908

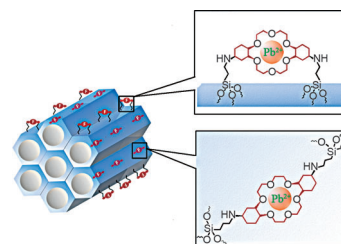


Mesoporous Materials

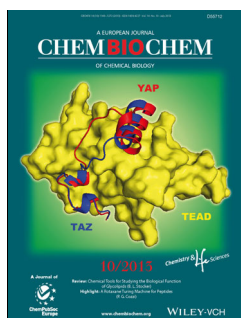
G. Ye,* Y. Leng, F. Bai, J. Wei, J. Wang, J. Chen*

Site-Selective Functionalization of Periodic Mesoporous Organosilica (PMO) with Macrocyclic Host for Specific and Reversible Recognition of Heavy Metal

Playing the host: A novel class of macrocyclic-host-functionalized periodic mesoporous organosilica (PMO) materials with excellent and reversible recognition of Pb^{II} was developed and upgraded by a site-selective post-modification method (see figure).



Chem. Asian J.
DOI: 10.1002/asia.201300131

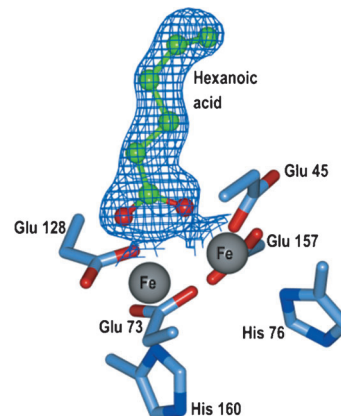


Decarbonylation

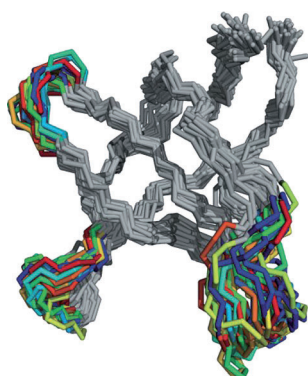
B. Khara, N. Menon, C. Levy, D. Mansell, D. Das, E. N. G. Marsh, D. Leys, N. S. Scrutton*

Production of Propane and Other Short-Chain Alkanes by Structure-Based Engineering of Ligand Specificity in Aldehyde-Deformylating Oxygenase

Biocatalytic propane production: structure-based engineering of aldehyde-deformylating oxygenase improves specificity for short- and medium-chain-length aldehydes and enhances the propane generation in whole-cell biotransformations. This presents new opportunities for developing biocatalytic modules for the production of volatile “drop-in” biofuels.

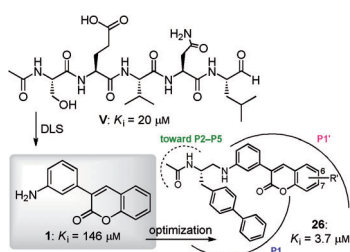


ChemBioChem
DOI: 10.1002/cbic.201300307



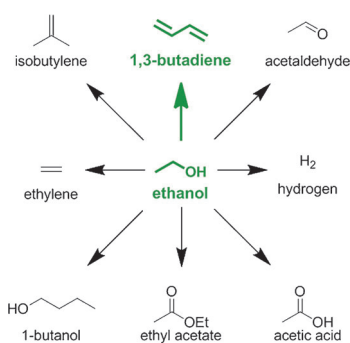
ChemPhysChem

DOI: 10.1002/cphc.201300377



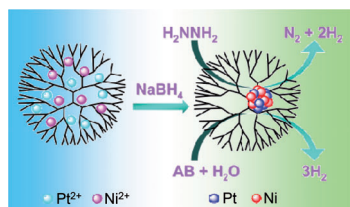
ChemMedChem

DOI: 10.1002/cmdc.201300078



ChemSusChem

DOI: 10.1002/cssc.201300214



ChemCatChem

DOI: 10.1002/cctc.201300143

Nuclear Magnetic Resonance

P. Guerry, L. Mollica, M. Blackledge*

Mapping Protein Conformational Energy Landscapes Using NMR and Molecular Simulation

A star is born: We present recent advances in the combination of NMR with state of the art molecular simulation that allows a detailed mapping of the protein conformational energy landscape. A novel combination of RDCs with accelerated molecular dynamics provides robust determination of ensemble representations of the underlying Boltzmann ensemble present in solution.

Fragment-Based Design

M. I. Fernández-Bachiller, A. Horatscheck, M. Lisurek, J. Rademann*

Alzheimer's Disease: Identification and Development of β -Secretase (BACE-1) Binding Fragments and Inhibitors by Dynamic Ligation Screening (DLS)

Fragment's guide to chemical space! Dynamic ligation screening (DLS) was applied successfully to an aspartic protease. A peptide aldehyde was used as a directing probe to pick inhibitory fragments for the S1' pocket of the aspartic protease BACE-1. The hit fragments can be extended into compounds containing the N-acylated ethane-1,2-diamine motif. The identified 3-(aminophenyl)coumarin fragment was set as a starting point for developing entirely nonpeptidic drug-like BACE-1 inhibitors with low-micromolar activity and the potential for further optimization.

Renewables

C. Angelici, B. M. Weckhuysen,* P. C. A. Bruijninx*

Chemocatalytic Conversion of Ethanol into Butadiene and Other Bulk Chemicals

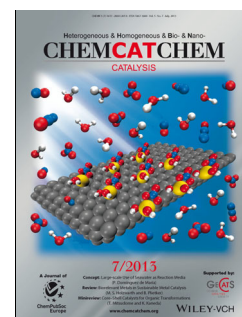
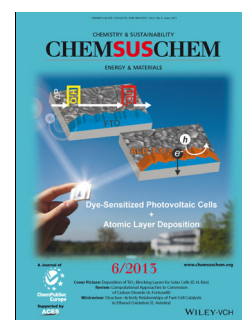
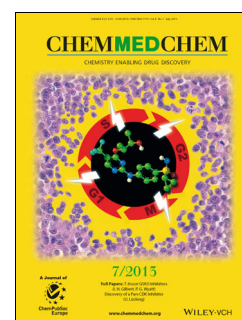
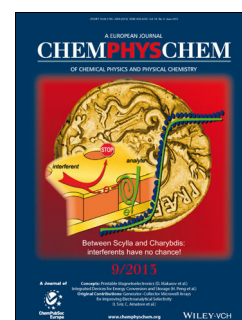
Fuel for thought: The dedicated production of 1,3-butadiene from bioethanol is expected to be an effective solution to its current substantial price increase. The Lebedev process for ethanol-to-butadiene conversion is reviewed in detail. The Review also extends to other commodity chemicals that are produced from ethanol and are involved as intermediates or byproducts in the bio-based butadiene production process.

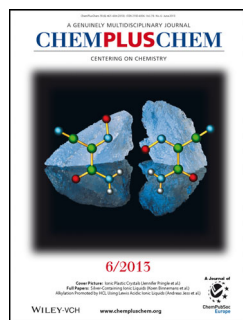
Dendrimers

K. Aranishi, A. K. Singh, Q. Xu*

Dendrimer-Encapsulated Bimetallic Pt-Ni Nanoparticles as Highly Efficient Catalysts for Hydrogen Generation from Chemical Hydrogen Storage Materials

I feel it in my dendrimers... Bimetallic Pt-Ni dendrimer-encapsulated nanoparticles (DENS) with different Pt/Ni ratios are synthesized through the co-complexation of Pt^{2+} and Ni^{2+} cations to the internal tertiary amine of the dendrimer followed by coreduction by $NaBH_4$. The Pt-Ni DENS show high catalytic activities in hydrous hydrazine decomposition and ammonia borane hydrolysis.



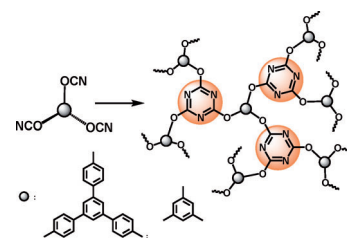


Mesoporous Materials

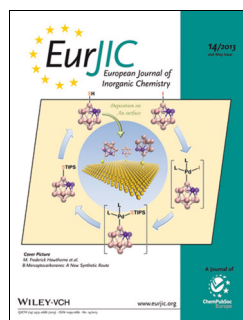
H. Yu, C. Shen, Z. Wang*

Micro- and Mesoporous Polycyanurate Networks Based on Triangular Units

Three sides to the story: Microporous and mesoporous polycyanurate networks were synthesized by means of thermal self-cyclotrimerization from two triangular cyanate resin monomers, 1,3,5-tri(4-cyanatophenyl)benzene and 1,3,5-tricyanatobenzene, respectively (see scheme). The adsorptions of CO₂, H₂, benzene, *n*-hexane, and water vapors were investigated.



ChemPlusChem
DOI: 10.1002/cplu.201300090

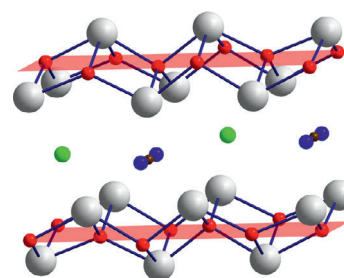


Luminescent Materials

M. Kubus,* D. Ensling, T. Jüstel, H.-J. Meyer*

A Luminescent Material: La₃Cl(CN₂)O₃:Ln 5 mol-% (Ln = Eu³⁺ or Tb³⁺ Ions

The new luminescent material La₃Cl(CN₂)O₃:Ln 5 mol-% (Ln = Eu³⁺ or Tb³⁺) was successfully synthesized by a simple reaction of LaOCl with Li₂CN₂ (+ LnCl₃).



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201300224

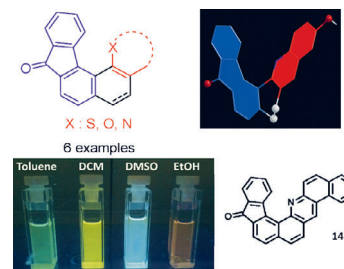


Heterocyclic Polycycles

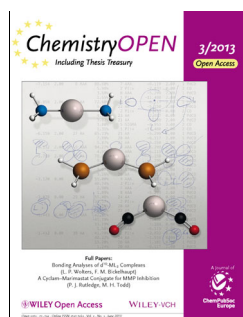
A. Souibgui, A. Gaucher, J. Marrot, F. Aloui, F. Mahuteau-Betzer, B. Ben Hassine,* D. Prim*

A Flexible Strategy Towards Thienyl-, Oxazolyl- and Pyridyl-Fused Fluorenones

Thienyl-, oxazolyl- and pyridyl-fused benzo[*c*]fluorenones were prepared from bromotetralone according to a flexible and short step strategy. The photophysical properties of the products depend on the nature of the fused heterocycle and are crucially influenced by structural modulations.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201300233

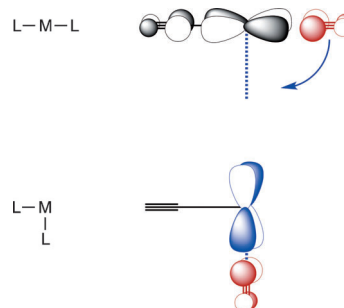


DFT Computations

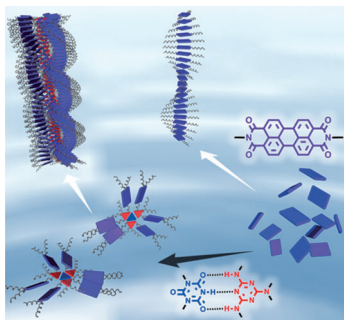
L. P. Wolters, F. M. Bickelhaupt*

Nonlinear d¹⁰-ML₂ Transition-Metal Complexes

π Electrons can do that! They can bend the otherwise linear d¹⁰-ML₂ complexes through backbonding. Bonding analyses reveal that the second π-accepting ligand is, in a sense, hunting for “fresh” (not yet stabilized) d_π electrons. The magnitude of the effect depends on the nature of both metal and ligand; L–M–L angles adopt values as small as 128.6°.



ChemistryOpen
DOI: 10.1002/open.201300009



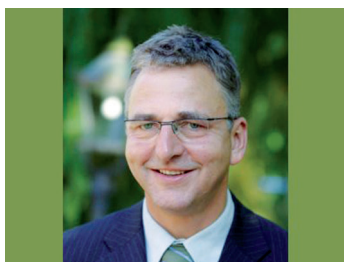
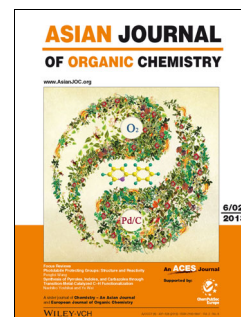
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201300025

Perylene Bisimides

T. Seki, X. Lin, S. Yagai*

Supramolecular Engineering of Perylene Bisimide Assemblies Based on Complementary Multiple Hydrogen Bonding Interactions

PBI Friday: Functional perylene bisimide assemblies that are constructed based on complementary multiple hydrogen-bonding interactions are reviewed. Supramolecular engineering of well-defined, hydrogen-bonded oligomers or polymers results in the formation of predictable extended assemblies through π - π stacking interactions. The unique optoelectronic and stimuli-responsive properties as well as the various morphologies of such assemblies are also introduced.



ChemViews magazine
DOI: 10.1002/chemv.201300065

Protein Engineering

Lisa-Marie Rauschendorfer

Uwe Bornscheuer on Biocatalysis and Publishing

The Co-Chairman of the Editorial Board of ChemCatChem, Professor Uwe Bornscheuer, talks in an interview about trends in his field of research, biocatalysis and protein engineering. He also explains why active engagement in publishing - as an author and an editor or publisher - is important for scientists.

