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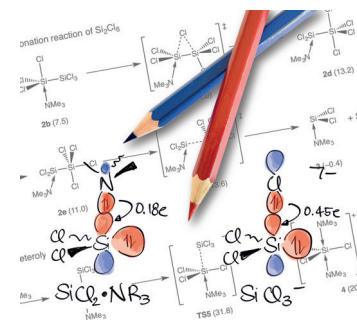


Density Functional Theory

J. I. Schweizer, L. Meyer, A. Nadj, M. Diefenbach, M. C. Holthausen*

Unraveling the Amine-Induced Disproportionation Reaction of Perchlorinated Silanes—A DFT Study

A neo twist: A DFT study on the amine-induced disproportionation reaction of Si_2Cl_6 to *neo*- $\text{Si}_5\text{Cl}_{12}$ discloses a stepwise rather than a concerted silylene insertion mechanism, which was generally accepted for over half a century. The resulting picture appears generalizable to the related chloride-induced chemistry recently explored (see graphic).



Chem. Eur. J.

DOI: 10.1002/chem.201602724

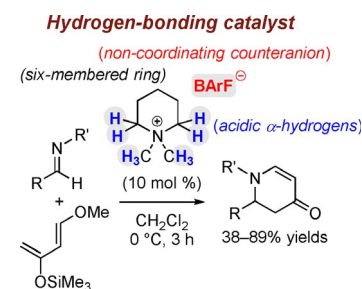


Aza-Diels–Alder Reactions

Y. Kumatabara, S. Kaneko, S. Nakata, S. Shirakawa,* K. Maruoka

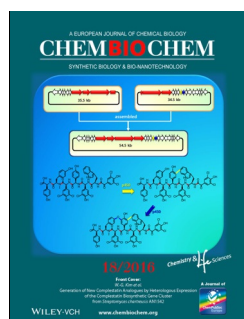
Hydrogen-Bonding Catalysis of Tetraalkylammonium Salts in an Aza-Diels–Alder Reaction

Under observation: A piperidine-derived tetraalkylammonium salt with a non-coordinating counteranion worked as an effective hydrogen-bonding catalyst in an aza-Diels–Alder reaction of imines and a Danishefsky diene. The hydrogen-bonding interaction between the ammonium salt and an imine was observed as part of a ^1H NMR titration study.



Chem. Asian J.

DOI: 10.1002/asia.201600781

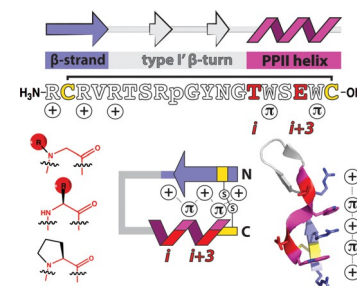


Peptidomimetics

T. W. Craven,* R. Bonneau, K. Kirshenbaum*

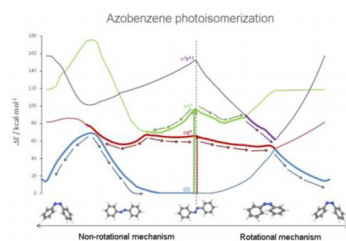
PPII Helical Peptidomimetics Templated by Cation– π Interactions

PPII helices on lockdown: A network of cation– π interactions was used to template peptide and peptoid residues into left-handed polyproline type II (PPII) helices, covalently locking the secondary structure with an engineered disulfide bridge. These chemically diverse PPII helical structures provide a new route toward peptidomimetic protein–protein interaction inhibitors.



ChemBioChem

DOI: 10.1002/cbic.201600248



ChemPhysChem

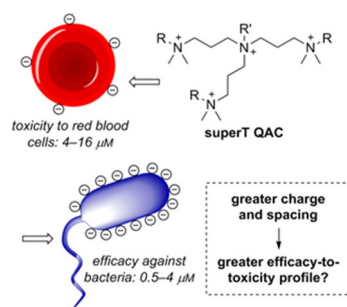
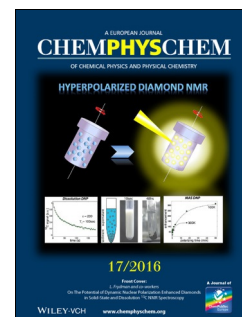
DOI: 10.1002/cphc.201600502

Photoisomerisation

J. Casellas, M. J. Bearpark, M. Reguero*

Excited-State Decay in the Photoisomerisation of Azobenzene: A New Balance between Mechanisms

Rotation versus inversion: The mechanism of photoisomerisation of azobenzene depends on the initial excitation and on the degree of constraint of the rotation of the system. Multiconfigurational ab initio calculations provide an accurate description of the potential energy surfaces of the excited states of this system when the dynamic electron correlation is included, and allow the experimental observations to be explained.



ChemMedChem

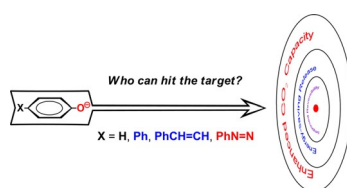
DOI: 10.1002/cmdc.201600176

Antibiotics

M. E. Forman, M. C. Jennings, W. M. Wuest,* K. P. C. Minbiole*

Building a Better Quaternary Ammonium Compound (QAC): Branched Tetracationic Antiseptic Amphiphiles

“SuperT” QACs: Disinfectants must have two key features: potent activity against a variety of microorganisms, and minimal toxicity to eukaryotic cells. How do we design nonspecific antibacterial agents that kill bacteria, yet are safe enough to use in households, hospitals, and industry? This work examines the role of charge and spacing in developing novel antiseptics with desirable efficacy to toxicity profiles.



ChemSusChem

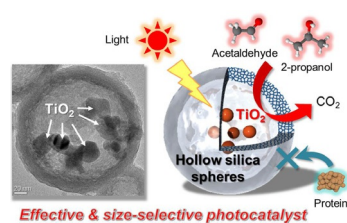
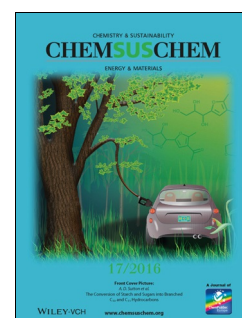
DOI: 10.1002/cssc.201600402

Carbon Dioxide Chemistry

M. Pan, N. Cao, W. Lin, X. Luo, K. Chen, S. Che, H. Li, C. Wang*

Reversible CO₂ Capture by Conjugated Ionic Liquids through Dynamic Covalent Carbon–Oxygen Bonds

Dual-tuning method: Through the introduction of a large π -conjugated structure into the anion, a dual-tuning approach to improve CO₂ capture by anion-functionalized ionic liquids (ILs) results in high capacities of up to 0.96 mol_{CO₂} mol_{IL}^{−1} and excellent reversibility. Quantum chemical calculations, spectroscopic investigations, and thermogravimetric analysis indicate that the increased capacity is a result of stronger dynamic covalent bonds.



ChemCatChem

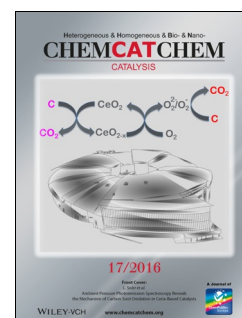
DOI: 10.1002/cctc.201600505

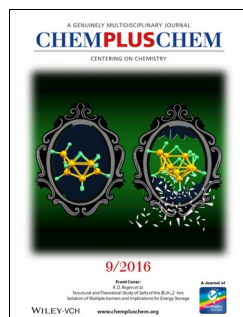
Photocatalysis

Y. Kuwahara, Y. Sumida, K. Fujiwara, H. Yamashita*

Facile Synthesis of Yolk–Shell Nanostructured Photocatalyst with Improved Adsorption Properties and Molecular-Sieving Properties

Oil in water for yolk in shell: A novel and facile method to fabricate yolk–shell nanostructured photocatalysts consisting of TiO₂ nanoparticles as the core and spherical hollow silica as the shell was developed. The yolk–shell nanostructures act as an efficient photocatalyst with both improved adsorption properties and molecular-sieving properties, which far outperformed those of naked TiO₂.



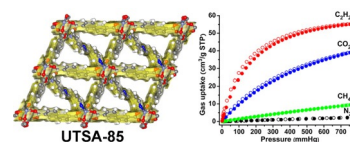


Metal–Organic Frameworks

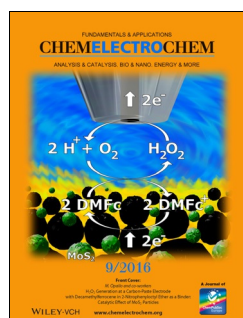
O. Alduhaish, H. Wang,* B. Li, H. D. Arman, V. Nesterov, K. Alfooty, B. Chen*

A Threefold Interpenetrated Pillared-Layer Metal–Organic Framework for Selective Separation of C_2H_2/CH_4 and CO_2/CH_4

Trapped wind: A new threefold interpenetrated pillared-layer microporous metal–organic framework, $[Zn_2(cca)_2(4-bpdb)]_n \cdot (DMF)_{2n}$ (UTSA-85) (H_2cca = 4-carboxycinnamic acid, 4-bpdb = 1,4-bis(4-pyridyl)-2,3-diaza-1,3-butadiene, and DMF = *N,N*-dimethylformamide), is described. The desolvated framework, UTSA-85a, exhibits high selectivity for C_2H_2/CH_4 separation as a result of the microporous structure and functional azine-groups decorating the pore channels (see figure).



ChemPlusChem
DOI: 10.1002/cplu.201600088

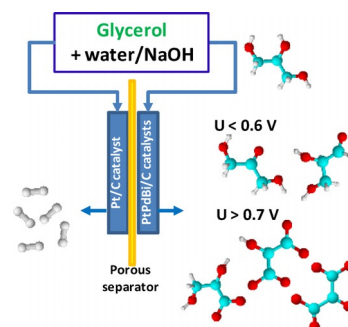


Nanocatalysts

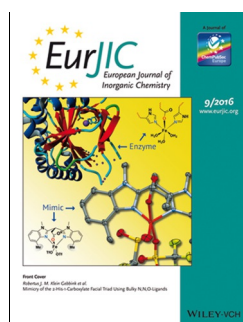
J. González-Cobos, S. Baranton, C. Coutanceau*

Development of Bismuth-Modified PtPd Nanocatalysts for the Electrochemical Reforming of Polyols into Hydrogen and Value-Added Chemicals

Bi adding value! Bismuth-modified PtPd anodes allow the production of hydrogen in an alkaline electrolysis cell at potentials as low as 0.3 V. Product identification by using FTIR spectroscopy indicates that glyceraldehyde and dihydroxyacetone are selectively formed at anode potentials lower than 0.55 V, whereas value-added C3 carboxylates are produced at anode potentials higher than 0.6 V. In addition, modification with bismuth avoids C–C bond breakage.



ChemElectroChem
DOI: 10.1002/celec.201600147

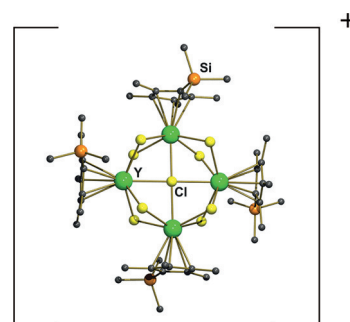


Olefin Polymerization

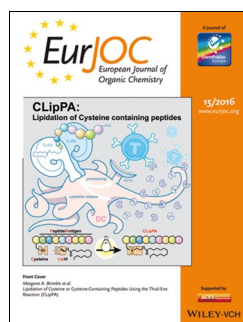
A. Fridrichová, V. Varga, J. Pinkas, M. Lamač, A. Růžicka, M. Horáček*

Yttrocene Chloride and Methyl Complexes with Various Substituted Cyclopentadienyl Ligands: Synthesis, Characterization, and Reactivity toward Ethylene

An ionic complex consisting of the tetranuclear anion $\{[(^5-C_5Me_4-SiMe_3)YCl_2]_4(\mu_4-Cl)^-\}$ and the thf-coordinated lithium cation $[Li(thf)_4]^+$ was used for the synthesis of mixed ytrocene chloride and methyl complexes containing two cyclopentadienyl ligands with different steric demands. Yttrocene methyl complexes were tested as catalysts in ethylene polymerization.



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201600390

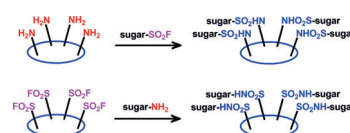


Sulfonamide Ligation

R. Zelli, S. Tommasone, P. Dumy, A. Marra,* A. Dondoni*

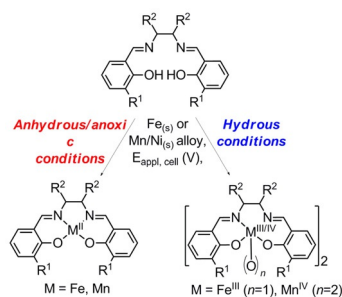
A Click Ligation Based on SuFEx for the Metal-Free Synthesis of Sugar and Iminosugar Clusters

The metal-free coupling between a tetra-aminated calixarene and a bench-stable C-glycosylsulfonamide gave the corresponding sugar cluster in good yield. The reversed sulfonamide bioisostere of the latter was prepared using a tetrasulfonamide calixarene and a C-glycosylalkylamine.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201600732

Electrosynthesis



ChemistryOpen

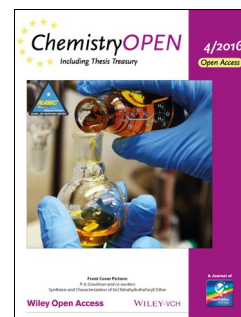
DOI: 10.1002/open.201600019

M. R. Chapman, S. E. Henkelis, N. Kapur, B. N. Nguyen,*
C. E. Willans*

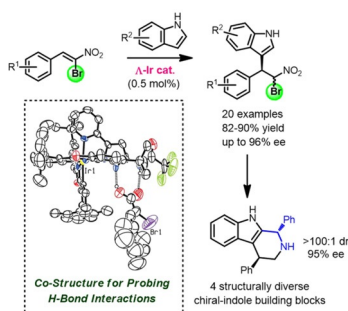
A Straightforward Electrochemical Approach to Imine- and Amine-bisphenolate Metal Complexes with Facile Control Over Metal Oxidation State

Smooth salen! Electrochemical synthesis has provided easy access to 34 complexes of diverse metal–ligand combinations. Facile control over metal oxidation state was possible through slight modification of reaction conditions.

Remarkably, selective metallation using a Mn/Ni alloy furnished analytically pure Mn complexes in high yield.



Asymmetric Catalysis

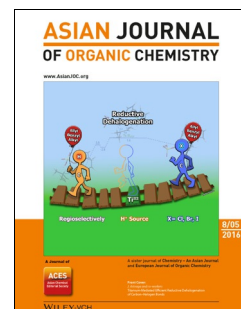


Asian J. Org. Chem.

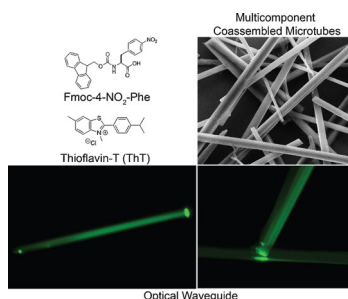
DOI: 10.1002/ajoc.201600288

K. Huang, Q. Ma, X. Shen, L. Gong,* E. Meggers*

Metal-Templated Asymmetric Catalysis: (Z)-1-Bromo-1-Nitrostyrenes as Versatile Substrates for Friedel–Crafts Alkylation of Indoles

An enantioselective Friedel–Crafts alkylation of indoles with α -bromo nitroalkenes has been developed by using a special metal-templated hydrogen-bonding complex. The mechanism involving multiple hydrogen-bonding interactions is well established by the co-crystal structure of a simplified iridium catalyst with a structural analog of the nitro substrate.

Molecular Assembly



ChemNanoMat

DOI: 10.1002/cnma.201600123

W. Liyanage, N. M. B. Cogan, B. L. Nilsson*

Amyloid-Inspired Optical Waveguides from Multicomponent Crystalline Microtubes

Follow the light: Crystalline microtubes formed by selective coassembly of amyloid-specific fluorophores and Fmoc-4-NO₂-Phe microtubes exhibit optical waveguide properties.

Photovoltaics



ChemViews magazine

DOI: 10.1002/chemv.201600064

T. Kueckmann, Q. Zhang

Electron Transport in Solar Cells

In “Behind the Science”, *ChemViews Magazine* gives readers a peek behind the scenes of a research article. This time, Theresa Kueckmann, *Chemistry—An Asian Journal*, talks to Qichun Zhang, Nanyang Technological University, Singapore, about his recent article on electron-transport layer materials for perovskite solar cells.