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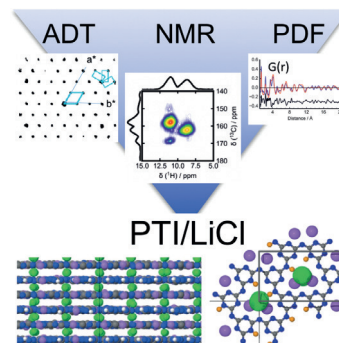


Structure Elucidation

M. B. Mesch, K. Bärwinkel, Y. Krysiak, C. Martineau, F. Taulelle, R. B. Neder,* U. Kolb,* J. Senker*

Solving the Hydrogen and Lithium Substructure of Poly(triazine imide)/LiCl Using NMR Crystallography

Methodological complementarity: The real structure of poly(triazine imide)/LiCl has finally been resolved based on a clever combination of multinuclear and multidimensional solid-state NMR spectroscopy, automated electron diffraction tomography, and an analysis of the X-ray pair distribution function (see graphic). Each method contributes with its individual strengths on different length scales, adding essential information to the complex structure-solution process.



Chem. Eur. J.
DOI: 10.1002/chem.201603726

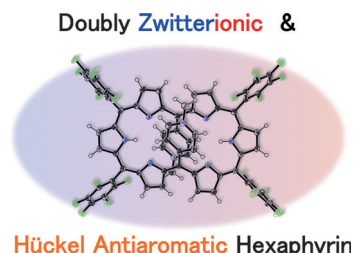


Hexaphyrins

K. Naoda, A. Osuka*

A Doubly Zwitterionic Antiaromatic [28]Hexaphyrin Formed upon Deprotonation of 5,20-Di(*N*-methyl-4-pyridinium)-Substituted [28]Hexaphyrin

Aromatic–Antiaromatic: A rectangular 5,20-di(4-pyridyl) [26]hexaphyrin was reduced with NaBH₄ to give the corresponding twisted Möbius aromatic [28]hexaphyrin. Subsequent double *N*-methylation gave a dicationic 5,20-di(*N*-methyl-4-pyridinium) [28]hexaphyrin, which was converted to a doubly zwitterionic Hückel antiaromatic [28]hexaphyrin upon deprotonation with sodium methoxide.



Chem. Asian J.
DOI: 10.1002/asia.201601071

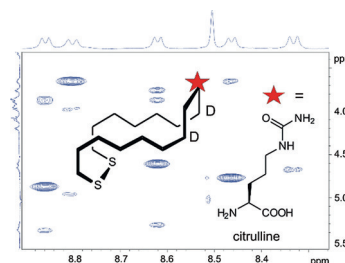


Peptidomimetics

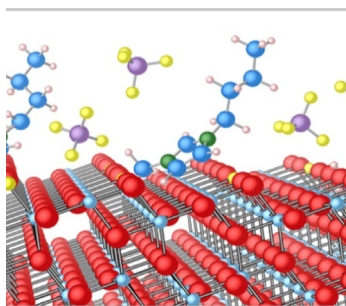
A. Schrimpf, A. Geyer*

Two Opposing D-Amino Acids Give Zigzag Hairpin Epitopes an Additional Kink to Create Antibody-Selective Peptide Antigens

Conformation determines activity: The zigzag shape of an all-L β-hairpin peptide is kinked by cross-strand correlated pairs of D-amino acids. The unusual epitope conformations were analyzed by NMR spectroscopy. These are specific synthetic antigens for antibody discrimination.



ChemBioChem
DOI: 10.1002/cbic.201600479



ChemPhysChem

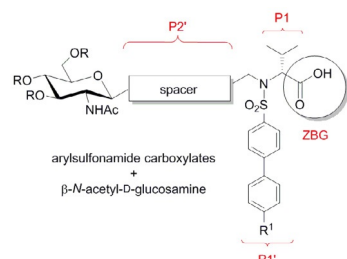
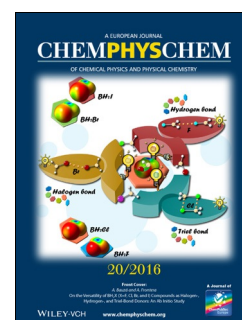
DOI: 10.1002/cphc.201600774

Ionic Liquids

M. Wagstaffe, M. J. Jackman, K. L. Syres, A. Generalov, A. G. Thomas*

Ionic Liquid Ordering at an Oxide Surface

The interaction of the ionic liquid $[C_4C_1Im][BF_4]$ with anatase TiO_2 , a model photoanode material, is studied using a combination of synchrotron radiation photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy.



ChemMedChem

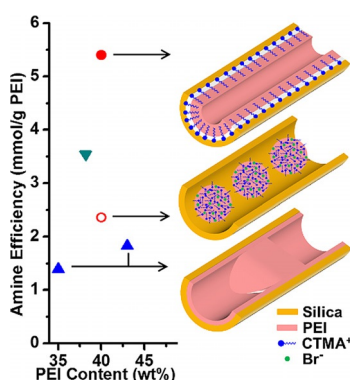
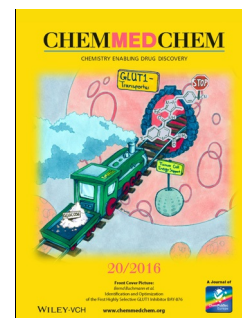
DOI: 10.1002/cmdc.201600235

Pulmonary and Cardiovascular Therapies

E. Nuti, D. Cuffaro, F. D'Andrea, L. Rosalia, L. Tepshi, M. Fabbj, G. Carbotti, S. Ferrini, S. Santamaria, C. Camodeca, L. Ciccone, E. Orlandini, S. Nencetti, E. A. Stura, V. Dive, A. Rossello*

Sugar-Based Arylsulfonamide Carboxylates as Selective and Water-Soluble Matrix Metalloproteinase-12 Inhibitors

Sugar power: Ten glycoconjugate arylsulfonamide carboxylates were designed and synthesized as matrix metalloproteinase-12 (MMP-12)-selective inhibitors with improved hydrophilicity. They were tested on recombinant MMPs by fluorimetric assays, and X-ray crystallographic studies helped rationalize the results. Introduction of β -N-acetyl-D-glucosamine at the P2' position was found to maintain nanomolar activity against MMP-12 and to boost bioavailability.



ChemSusChem

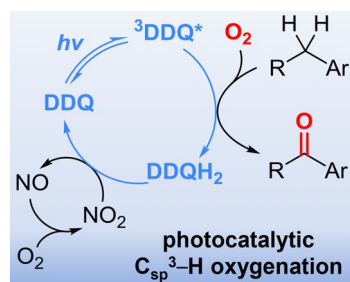
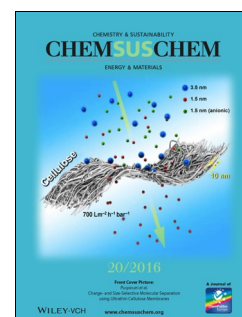
DOI: 10.1002/cssc.201600834

Carbon Capture

A. Sayari,* Q. Liu, P. Mishra

Enhanced Adsorption Efficiency through Materials Design for Direct Air Capture over Supported Polyethylenimine

Catch CO₂ if you can: Supported polyethylenimine (PEI) adsorbents with unprecedented amine efficiencies are obtained for the capture of CO₂ from air through molecular-scale design. A uniform layer of cetyltrimethylammonium (CTMA⁺) cations over the internal surface of the silica support plays a key role in the distribution of PEI throughout the extra-large pore channels and, thus, promotes CO₂ interactions with amine groups.



ChemCatChem

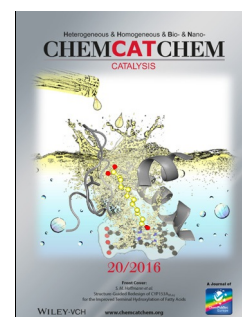
DOI: 10.1002/cctc.201600704

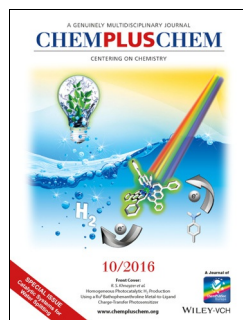
Photocatalysis

F. Rusch, J.-C. Schober, M. Brasholz*

Visible-Light Photocatalytic Aerobic Benzylic C(sp³)–H Oxygenations with the ³DDQ*/tert-Butyl Nitrite Co-catalytic System

DDQ can do: Visible-light-induced aerobic C(sp³)–H oxygenations of benzylic substrates are efficiently performed by using a co-catalytic system of ³DDQ* (DDQ = 2,3-dichloro-5,6-dicyano-1,4-benzoquinone) and tert-butyl nitrite. The photocatalytic method offers a dramatic increase in reaction rate compared to the thermal protocol.



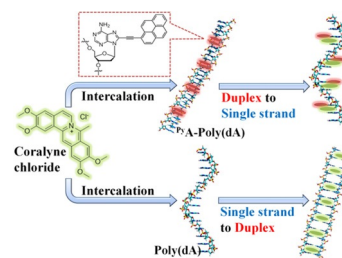


DNA Duplexes

K. T. Kim, T. S. Choi, K. Y. Kim, H. I. Kim, B. H. Kim*

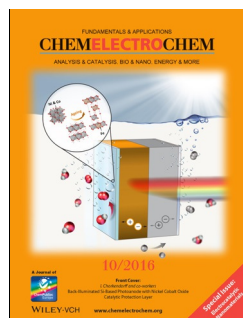
Disassembly of Chromophore-Guided DNA Duplexes through Site-Selective Binding of Coralyne to Pyrene-Modified Adenine Bases

Intercalation for separation: Disassembly of chromophore-guided DNA assemblies carried out under ambient temperature has been achieved through intercalative binding of coralynes to pyrene-modified adenine (^PA) bases (see figure). This behavior, which is opposite to that of coralyne-induced self-duplex formation of natural oligodeoxyadenylates, was applied to prepare new types of coralyne-stimulated switchable DNA modules.



ChemPlusChem

DOI: 10.1002/cplu.201600230

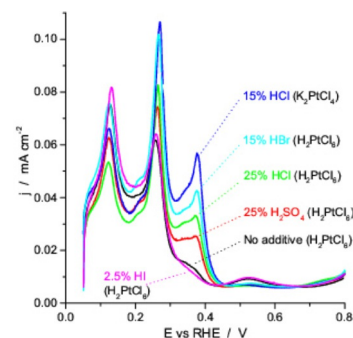


Nanoparticles

R. A. Martínez-Rodríguez, F. J. Vidal-Iglesias, J. Solla-Gullón, C. R. Cabrera, J. M. Feliu*

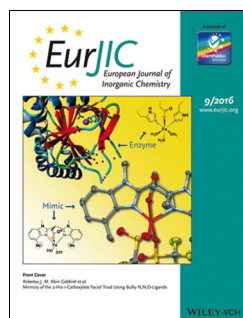
Electrochemical Characterisation of Platinum Nanoparticles Prepared in a Water-in-Oil Microemulsion in the Presence of Different Modifiers and Metal Precursors

Get in shape: Pt nanoparticles prepared in water-in-oil microemulsions in the presence of different surface modifiers are electrochemically characterized. Well-defined cubic nanoparticles with a preferred (100) surface structure are obtained and tested in different electrocatalytic reactions.



ChemElectroChem

DOI: 10.1002/celec.201600295

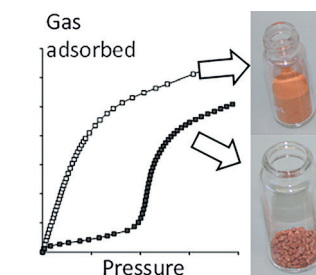


Gas Adsorption

N. Chanut, A. D. Wiersum, U.-H. Lee, Y. K. Hwang, F. Ragon, H. Chevreau, S. Bourrelly, B. Kuchta, J.-S. Chang, C. Serre, P. L. Llewellyn*

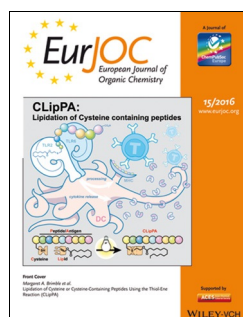
Observing the Effects of Shaping on Gas Adsorption in Metal-Organic Frameworks

A series of four metal-organic frameworks were synthesized as powders and spheres, and these were characterized by gas adsorption at 30 °C coupled with microcalorimetry. Whereas most variations were expected, interesting effects including partial pore restriction and active site "protection" were also evidenced for some shaped materials, suggesting that the binder may play a more complex role.



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201600410

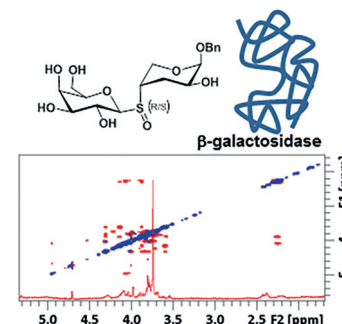


Glycomimetics

J. P. Colomer, B. Fernández de Toro, F. J. Cañada, F. Corzana, J. Jiménez Barbero,* Á. Canales,* O. Varela*

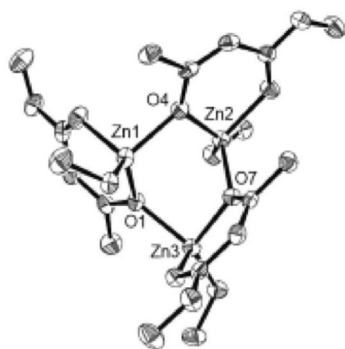
Diastereomeric Glycosyl Sulfoxides Display Different Recognition Features versus *E. coli* β -Galactosidase

The saccharide mimicry is an essential part of the development of sugar-based drugs and/or molecular probes. In this work we characterize the conformational behavior of a glycosyl sulfoxide and its interaction with *E. coli* β -galactosidase, by using NMR spectroscopy; (*S*) and (*R*) diastereoisomers of the sulfoxide could be analyzed, and each diastereomer displays a different potency as an enzyme inhibitor.



Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201600835



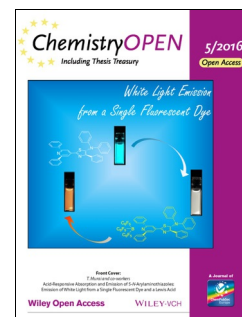
ChemistryOpen
DOI: 10.1002/open.201600040

Structure Elucidation

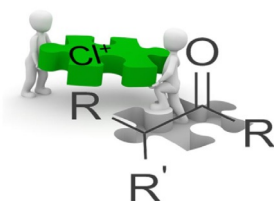
J. A. Manzi, C. E. Knapp, I. P. Parkin, C. J. Carmalt*

Synthesis of Trimeric Organozinc Compounds and their Subsequent Reaction with Oxygen

Cycle route: A cyclic trimeric organozinc compound of the type $[\{Zn(Et)(\beta\text{-diketonate})\}_3]$ is described and structurally characterized for the first time. The selective oxidation of species of this type produces $[\{Zn(\beta\text{-diketonate})_2Zn(Et)OEt\}_2]$, allowing a high oxygen content, structural stability, and suitability as precursors to zinc oxide thin films through aerosol-assisted chemical vapor deposition (AACVD).



Asymmetric Organocatalysis



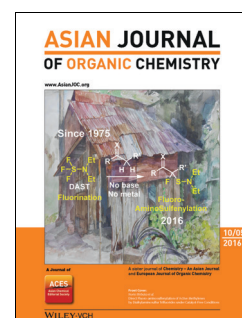
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201600404

Asymmetric Organocatalysis

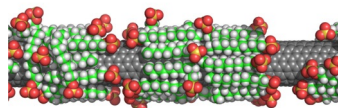
M. Gómez-Martínez, D. A. Alonso, I. M. Pastor, G. Guillena, A. Baeza*

Organocatalyzed Assembly of Chlorinated Quaternary Stereogenic Centers

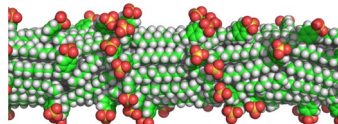
The missing piece: The construction of chlorinated quaternary stereocenters is a challenge for organic chemists. The growth in organocatalysis has prompted the exploration of such a strategy for this purpose. This review focuses on state-of-the-art research in the area of organocatalysis for the construction of chlorinated quaternary stereocenters and presents both successful examples and limitations that still need to be overcome.



SDS



SDBS



ChemNanoMat
DOI: 10.1002/cnma.201600190

Redox Chemistry of Nanotubes

A. Hirano,* T. Kameda, Y. Yomogida, M. Wada, T. Tanaka, H. Kataura

Origin of the Surfactant-Dependent Redox Chemistry of Single-Wall Carbon Nanotubes

Surfactant-dependent redox chemistry: Sodium dodecyl sulfate (SDS) forms single layers on single-walled carbon nanotubes (SWCNTs) with solvent-exposed areas, whereas sodium dodecylbenzenesulfonate (SDBS) densely coats the SWCNTs. The SDBS layer on the SWCNT surfaces prevents charge-transfer reactions. A positively charged SWCNT as a model of the oxidized SWCNT showed an increase in the number of surfactant molecules around the SWCNT in the SDS solution through electrostatic interactions.



ChemViews magazine
DOI: 10.1002/chemv.201600071

Career

L. Bohn, R. Threlfall

Career: As a Chemist Managing Products

In an interview series, *ChemistryViews.org* gives readers a glimpse into the wide range of career paths in chemistry. This time, Dr. Richard Threlfall, Product Manager for Wiley Science Solutions, talks about his job. He sees scientists as problem solvers who can adapt to different tasks in the workplace and explains why he considers *ChemPlanner* a game-changing software for synthesis planning.

