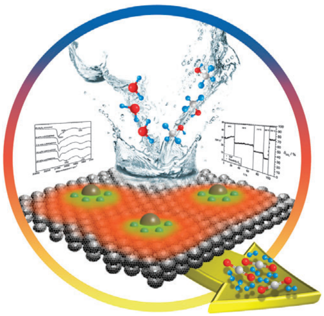
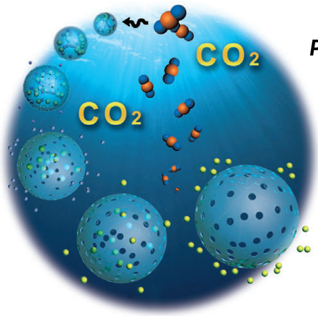
The benzene dimer …

… has an asymmetric T-shaped equilibrium structure but exhibits the rotational spectrum of a symmetric top with a rich substructure. In their experimental and theoretical study on page 5180 ff., A. Schnell, A. van der Avoird, and co-workers show that this substructure arises from a concerted sixfold rotation tunneling of the unit in the stem and tilt tunneling of the unit in the cap. The unexpected symmetric-top spectrum results from nearly free rotation of the cap.

Heterogeneous Catalysis

In their Communication on page 5028 ff., P. Wasserscheid and co-workers describe a Pt–alumina catalyst whose surface is modified with alkali-metal salt coatings. The resulting catalyst is highly active and selective for the methanol steam reforming reaction.



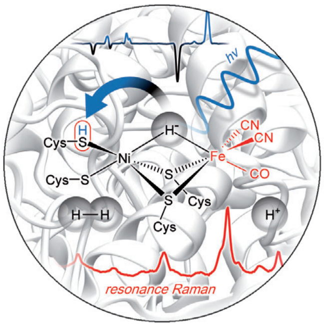


Polymersomes

In their Communication on page 5070 ff., J. Y. Yuan et al. describe the use of CO_2-sensitive block copolymers to build biomimetic sacs in which the membrane pores can be tuned by controlling CO_2 levels.

Hydrogenases

In their Communication on page 5162 ff. P. Hildebrandt, I. Zebger, M. Horch, and co-workers use resonance Raman spectroscopy to obtain new insights into the structure and photochemical properties of the active centers of [NiFe] hydrogenases.



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Service

Author Profile

"My favorite composer is Johann Sebastian Bach. My favorite time of day is after dinner, because I can relax. …"
This and more about Nagao Kobayashi can be found on page 4980.

News

K. Müller

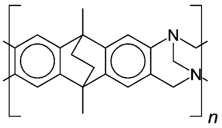
W. Bonrath

M. Rogers-Evans

R. S. Langer

Highlights

Gas Separation



PIM-EA-TB

On the way to membranes for the separation of industrially important gas pairs, researchers have devised the new ladder polymer PIM-EA-TB, which was found to have remarkable selectivity and permeability for several technically relevant gas pairs. A possible explanation of these observations is given.

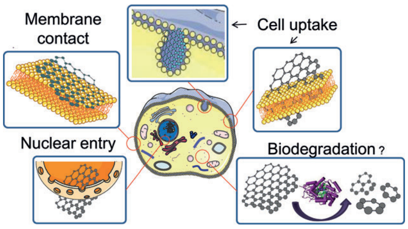
Minireviews

Nanomaterials

A. Bianco* ______ **4986 – 4997**

Graphene: Safe or Toxic? The Two Faces of the Medal

Two sides of the coin: Graphene is part of a bigger family identified as the graphene family nanomaterials (GFNs). For their development, it is important to evaluate the safety profiles and impacts on health. Some studies clearly show no particular risks exist and others indicate that GFNs might become health hazards.



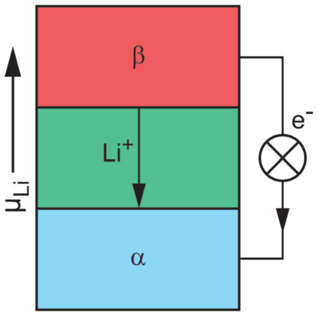
Reviews

Lithium Batteries

J. Maier* ______ **4998 – 5026**

Thermodynamics of Electrochemical Lithium Storage

No defects, no equilibrium: The equilibrium properties of electrochemical storage of lithium in solids are treated bearing in mind that defects in solids are the mechanistically relevant centers. Nanomaterials and amorphous materials are dealt with in the context of constrained equilibria. Finally, it is shown that the application of defect chemistry also allows for a pertinent thermodynamic treatment of interfacial storage.



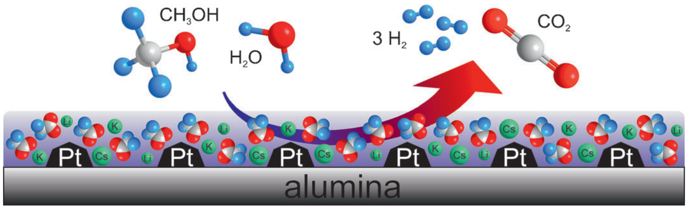
Communications

Heterogeneous Catalysis

M. Kusche, F. Enzenberger, S. Bajus,
H. Niedermeyer, A. Bösmann, A. Kaftan,
M. Laurin, J. Libuda,
P. Wasserscheid* ______ **5028 – 5032**

Enhanced Activity and Selectivity in Catalytic Methanol Steam Reforming by Basic Alkali Metal Salt Coatings

Frontispiece



Tri-salts added: Pt on alumina catalysts can be used for converting methanol and water into hydrogen and carbon dioxide (see picture), for applications such as hydrogen storage. Both the activity and selectivity could be enhanced by coating these materials with a thin layer of a molten salt mixture of Li/K/Cs acetate. Potassium doping was identified by DRIFTS measurements to be an important factor for the boost in catalyst performance.

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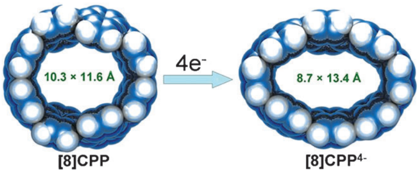
Charged Nanobelts

A. V. Zabula, A. S. Filatov, J. Xia, R. Jasti,*
M. A. Petrukhina* — 5033 – 5036

Tightening of the Nanobelt upon Multielectron Reduction

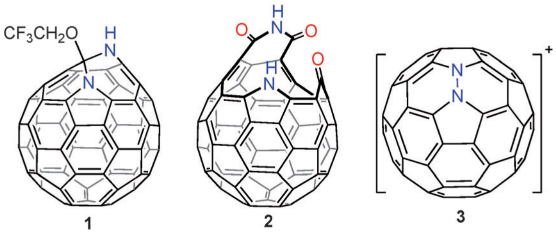


A painless way to tighten your belt: Structural characterization of the multiply charged fragment of an armchair nanotube that was formed by reduction of the neutral molecule with potassium metal revealed a remarkable elliptical distortion of the carbon core (see picture). The resulting tetraanions underwent supramolecular aggregation with potassium cations, and solvated guests were encapsulated inside the negatively charged polyarene cavity.

Heterofullerenes

H. Huang, G. H. Zhang, D. Wang,
N. N. Xin, S. S. Liang, N. D. Wang,
L. B. Gan* — 5037 – 5040

Synthesis of an Azahomoazafullerene $C_{59}N(NH)R$ and Gas-Phase Formation of the Diazafullerene $C_{58}N_2$

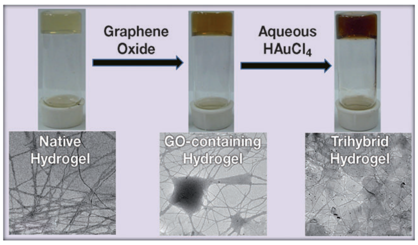


Open the cage if you dare: The azahomoazafullerene **1** was prepared from a *tert*-butylperoxy-substituted azafullerene derivative $C_{59}NBr(OOtBu)_4$. Singlet oxygen added to **1** to form an open-cage azafullerene **2** with a ketoimide moiety on the rim of the orifice. The MALDI-TOF mass spectrum of the product of the hydrolysis of **1** showed a clear signal for the diazafullerene $C_{58}N_2$ (see structure **3**).

Soft Matter

J. Nanda, A. Biswas, B. Adhikari,
A. Banerjee* — 5041 – 5045

A Gel-Based Trihybrid System Containing Nanofibers, Nanosheets, and Nanoparticles: Modulation of the Rheological Property and Catalysis

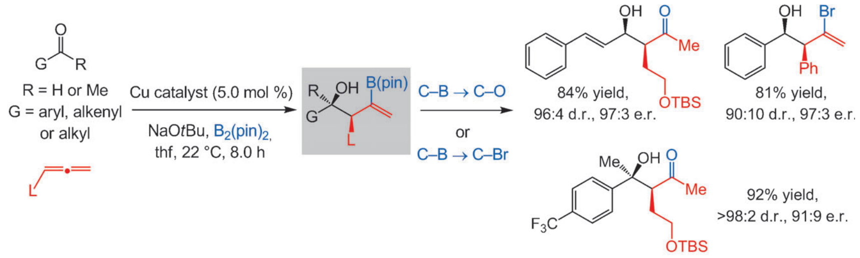


Wonderful gels: A trihybrid gel was prepared by incorporating graphene oxide and in situ synthesized gold nanoparticles (AuNPs) into an amino-acid-based native gel matrix (see pict). The morphology of this system indicates the presence of three distinctly different nanostructures: nanofibers, nanosheets, and nanoparticles. The catalytic efficiency of this trihybrid system is enhanced relative to that of AuNPs in a dihybrid system.

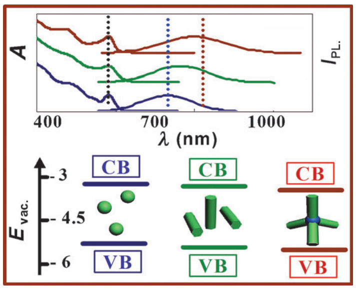
Multicomponent Reactions

F. Meng, H. Jang, B. Jung,
A. H. Hoveyda* — 5046 – 5051

Cu-Catalyzed Chemoselective Preparation of 2-(Pinacolato)boron-Substituted Allylcopper Complexes and their In Situ Site-, Diastereo-, and Enantioselective Additions to Aldehydes and Ketones



Sustainable, efficient, selective: A three-component, single-vessel Cu-catalyzed method for chemo-, diastereo-, and enantioselective conversion of $B_2(pin)_2$, monosubstituted allenes, and aldehydes or ketones to 2-B(pin)-substituted homoallylic alkoxides is described. Subsequent functionalization delivers valuable products in up to > 98:2 d.r. and 97:3 e.r. (see scheme).



Energy levels of semiconductor NCs are vital important for rational design of the nanodevices fabricated by using the NCs as building blocks. An approach for determining the energy levels was developed by introduction of transition-metal ions as dopants. The difference in the energy levels of the NCs with different composition, sizes, and shapes could be clearly revealed by such an approach. CB = conduction band, VB = valence band.

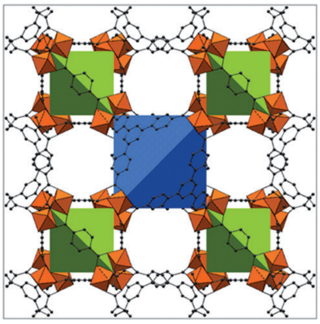
Nanocrystals

Z. L. Zhang, D. Z. Li, R. G. Xie,*
W. S. Yang ——— **5052 – 5055**

Insights into the Energy Levels of Semiconductor Nanocrystals by a Dopant Approach

---

It's all in the mix! Metal–organic frameworks (MOFs) were constructed from iron(III) trimers and mixtures of di- and tricarboxylate linkers. The dicarboxylate linker determined the size and shape of the pores in one series of materials with an interwoven structure and also enabled the introduction of different functionalities. Another mesoporous iron(III) MOF based on hybrid supertetrahedra had an extended β-cristobalite structure (see picture).

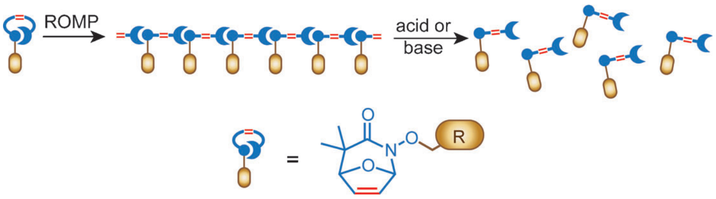


Porous Coordination Polymers

H. Chevreau, T. Devic,* F. Salles,
G. Maurin, N. Stock,
C. Serre* ——— **5056 – 5060**

Mixed-Linker Hybrid Superpolyhedra for the Production of a Series of Large-Pore Iron(III) Carboxylate Metal–Organic Frameworks

---



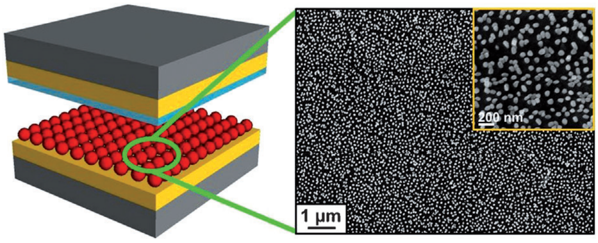
ROMP: A heterobicyclic olefin containing an oxazinone core is a new substrate for the ring-opening metathesis polymerization (ROMP). The polymers produced undergo degradation when exposed to either acidic or basic conditions. Furthermore, a monomer that can be readily diversified to access degradable polymers bearing tailored functionality was developed.

Polymers

J. M. Fishman,
L. L. Kiessling* ——— **5061 – 5064**

Synthesis of Functionalizable and Degradable Polymers by Ring-Opening Metathesis Polymerization

---



Moving to mercury: The first triboelectric effect-based sensor for the detection of Hg^{2+} ions by using Au nanoparticles (see picture; red) as electrical performance enhancer and recognition element has been successfully demonstrated. This self-powered and stand-alone triboelectric nanosensor has the advantages of simplicity, low cost, high selectivity, and sensitivity.

Triboelectric Nanosensors

Z.-H. Lin, G. Zhu, Y. S. Zhou, Y. Yang,
P. Bai, J. Chen, Z. L. Wang* **5065 – 5069**

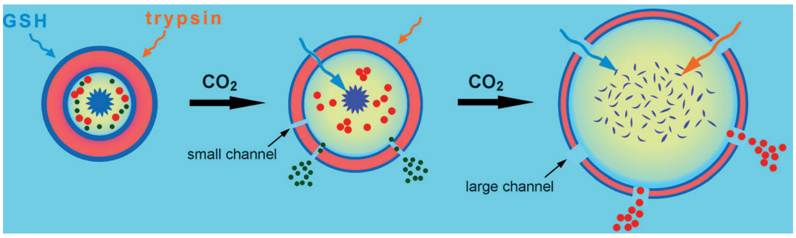
A Self-Powered Triboelectric Nanosensor for Mercury Ion Detection

Polymersomes

Q. Yan, J. B. Wang, Y. W. Yin, J. Y. Yuan* ______ 5070–5073

Breathing Polymersomes: CO_2-Tuning Membrane Permeability for Size-Selective Release, Separation, and Reaction

Inside Back Cover

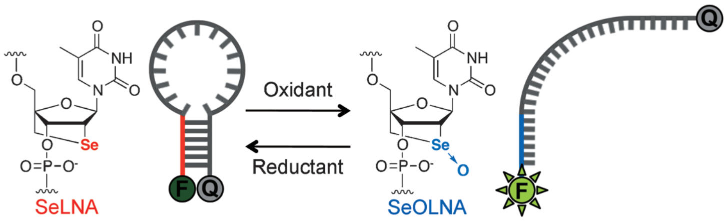


Take a deep breath: The membrane permeability and the scale of membrane nanochannels of polymer vesicles are modulated by CO_2 control of vesicular expansion and contraction. These polymersomes can act as size-selective nanoseparators for particle sieving and as nanoreactors for enzymatic reactions that require compartmentalization. GSH = glutathione.

Nucleic Acid Modifications

K. Morihiro, T. Kodama, Kentefu, Y. Moai, R. N. Veedu, S. Obika* ______ 5074–5078

Selenomethylene Locked Nucleic Acid Enables Reversible Hybridization in Response to Redox Changes

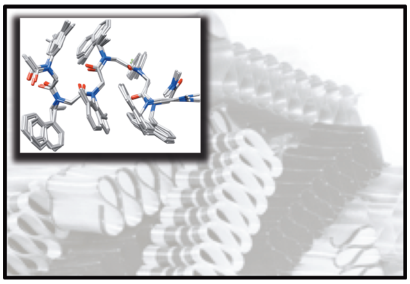


Locking up selenium: A new conformationally restricted nucleic acid with a 2′,4′-selenomethylene bridge (SeLNA) can be reversibly converted into its oxidized form (SeOLNA), and the hybridization of a modified oligonucleotide was shown to be dependent on the oxidation state. A SeLNA-modified molecular-beacon-type probe (see scheme; F = fluorophore, Q = quencher) can be used as a sensor for changes in the redox environment.

Peptoid Foldamers

J. A. Crapster, I. A. Guzei, H. E. Blackwell* ______ 5079–5084

A Peptoid Ribbon Secondary Structure



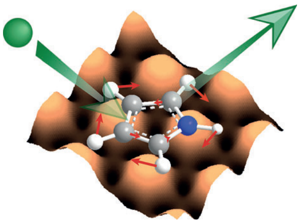
Joining the fold: A series of peptoids, or oligomers of *N*-substituted glycines, adopt a novel secondary structure, designated the "peptoid ribbon". This fold was stable at short chain lengths and in a variety of solvents (both organic and aqueous), and arose from a primary sequence of peptoid monomers designed to enforce an alternating pattern of *cis* and *trans* main-chain amides.

Surface Quantum Dynamics

B. A. J. Lechner,* H. Hedgeland, J. Ellis, W. Allison, M. Sacchi, S. J. Jenkins, B. J. Hinch ______ 5085–5088

Quantum Influences in the Diffusive Motion of Pyrrole on Cu(111)

Inside Cover

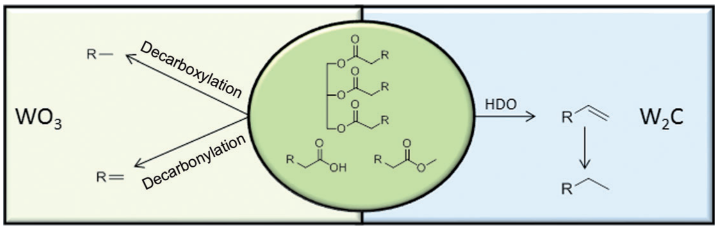


Classical diffusion—quantum barrier: On Cu(111), pyrrole diffuses in channels, hopping between adjacent bridge sites over a barrier above hollow sites. The motion of the center of mass can be described classically; however, the activation barrier arises from the quantum character of internal vibrational modes that are largely unexcited during the motion. The unique helium spin-echo experiment is indicated by the green sphere and arrows.

Biomass

R. W. Gosselink, D. R. Stellwagen,
J. H. Bitter* ______________ **5089 – 5092**

Tungsten-Based Catalysts for Selective Deoxygenation

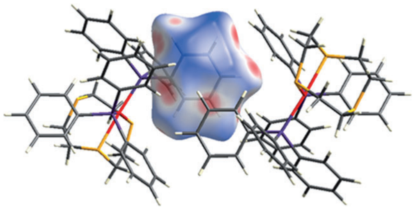


On the tip of the tung(sten): The title catalysts selectively perform deoxygenation of vegetable-oil-based feeds by either decarboxylation/decarbonylation or hydrodeoxygenation (HDO) pathways, depending on the dominant tungsten phase (WO$_3$ and W$_2$C). The process upgrades vegetable-oil-based feeds, under a hydrogen atmosphere, to high-value olefinic products, thus providing a significant advantage over other types of deoxygenation catalysts.

Structure Determination

H. L. S. Wong, D. R. Allan,
N. R. Champness, J. McMaster,
M. Schröder,* A. J. Blake* __ **5093 – 5095**

Bowing to the Pressure of π⋯π Interactions: Bending of Phenyl Rings in a Palladium(II) Thioether Crown Complex

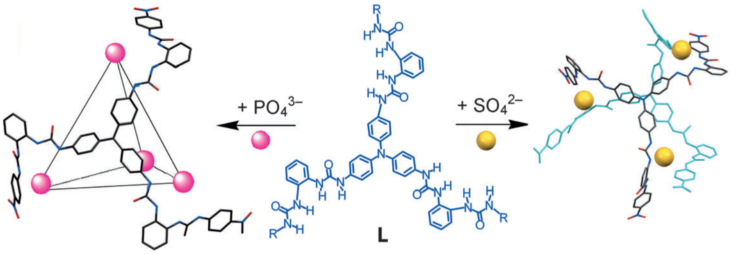


Compression of a parallel four-fold phenyl embrace involving two cations in $[Pd([9]aneS_3)(PPh_3)_2](PF_6)_2$ ($[9]aneS_3 =$ 1,4,7-trithiacyclononane) leads to π⋯π stacking interactions and concomitant pyramidalization at the *ipso* carbon atom of one of the phenyl rings. These pressure-induced transformations have been rationalized by Hirshfeld surface analysis, density functional calculations and natural bond orbital analysis.

Anion Coordination

B. Wu,* F. Cui, Y. Lei, S. Li, N. S. Amadeu,
C. Janiak, Y.-J. Lin, L.-H. Weng, Y.-Y. Wang,
X.-J. Yang ______________ **5096 – 5100**

Tetrahedral Anion Cage: Self-Assembly of a $(PO_4)_4L_4$ Complex from a Tris(bisurea) Ligand

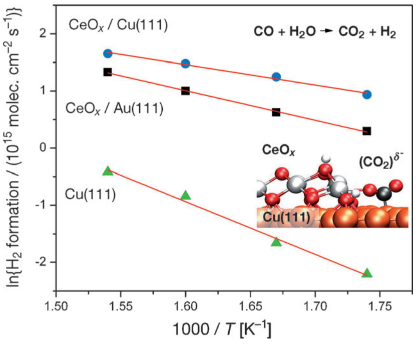


A C_3-symmetric tris(bisurea) ligand **L** assembles with PO_4^{3-} ions to form the tetrahedral cage $[(PO_4)_4\mathbf{L}_4]^{12-}$. The PO_4^{3-} ions form the four vertices and each forms 12 N—H⋯O hydrogen bonds with 6 urea groups. A unique trinuclear pinwheel-like helical complex $[(SO_4)_3\mathbf{L}_2]^{6-}$ is formed from **L** and SO_4^{2-} ions (see picture).

Heterogeneous Catalysis

K. Mudiyanselage, S. D. Senanayake,
L. Feria, S. Kundu, A. E. Baber, J. Graciani,
A. B. Vidal, S. Agnoli, J. Evans, R. Chang,
S. Axnanda, Z. Liu, J. F. Sanz, P. Liu,
J. A. Rodriguez,
D. J. Stacchiola* __________ **5101 – 5105**

Importance of the Metal–Oxide Interface in Catalysis: In Situ Studies of the Water–Gas Shift Reaction by Ambient-Pressure X-ray Photoelectron Spectroscopy

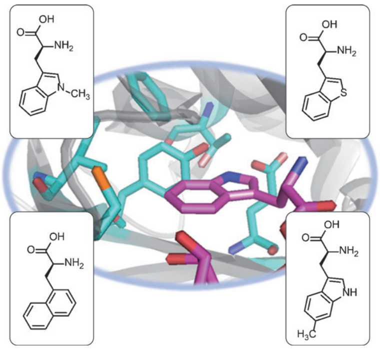


Where oxide and metals meet: The activation of an efficient associative mechanistic pathway for the water–gas shift reaction by an oxide–metal interface leads to an increase in the catalytic activity of nanoparticles of ceria deposited on Cu(111) or Au(111) by more than an order of magnitude (see graph). In situ experiments demonstrated that a carboxy species formed at the metal–oxide interface is the critical intermediate in the reaction.

Genetic Codon Expansion

A. Chatterjee, H. Xiao, P. Y. Yang,
G. Soundararajan,
P. G. Schultz* ________ 5106–5109

A Tryptophanyl-tRNA Synthetase/tRNA Pair for Unnatural Amino Acid Mutagenesis in *E. coli*

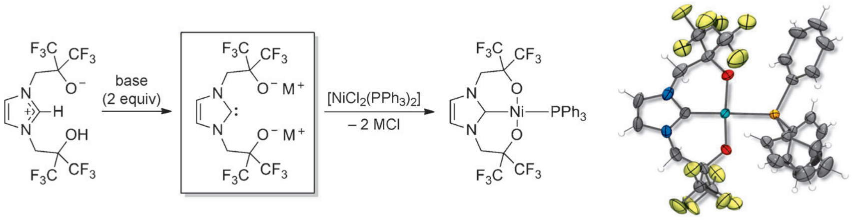


Selected: A tryptophanyl-tRNA synthetase(TrpRS)/tRNA pair was evolved to genetically encode tryptophan analogues and other unnatural amino acids with large side chains in *E. coli*. A selection scheme was employed to identify TrpRS variants able to selectively charge $\text{tRNA}_{\text{CUA}}^{\text{Trp}}$ with Trp analogues (see picture). Substitution of Trp66 in enhanced cyan fluorescent protein (ECFP) with these Trp analogues afforded ECFP variants with novel spectral properties.

Fluorinated Ligands

A. J. Arduengo, III,* J. S. Dolphin,
G. Gurău, W. J. Marshall, J. C. Nelson,
V. A. Petrov, J. W. Runyon* _ 5110–5114

Synthesis and Complexes of Fluoroalkoxy Carbenes

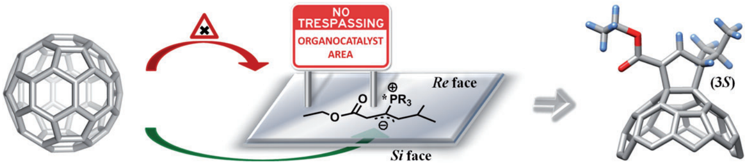


Gripping ligands: A series of fluoroalkoxy-functionalized imidazol-2-ylidene ligands were synthesized by the alkylation of a range of commercially available azoles with hexafluoroisobutylene oxide. The deprotonation of these species with a strong base cleanly generated the free carbenes, which acted as tridentate chelating ligands (see scheme).

Fullerenes

J. Marco-Martínez, V. Marcos,
S. Reboredo, S. Filippone,
N. Martín* ________ 5115–5119

Asymmetric Organocatalysis in Fullerenes Chemistry: Enantioselective Phosphine-catalyzed Cycloaddition of Allenoates onto C_{60}



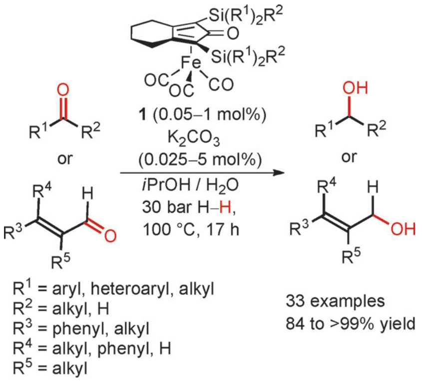
Organocatalysis and fullerenes merge: The first asymmetric organocatalytic synthesis by phosphine-catalyzed [3+2] cycloaddition of allenoates onto [60]fullerene that occurs under mild conditions giving rise to enantiomerically pure carbocyclic fullerene derivatives is reported. X-ray analysis of a cyclopenteno[60]fullerene has allowed the assignment of the absolute configuration of the new stereocenter. Furthermore, the sector rule previously used to assign the chirality in [60]fullerenes has been corrected in the light of these new experimental findings.

Reduction

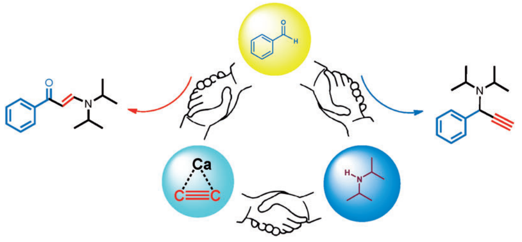
S. Fleischer, S. Zhou, K. Junge,
M. Beller* ________ 5120–5124

General and Highly Efficient Iron-Catalyzed Hydrogenation of Aldehydes, Ketones, and α,β-Unsaturated Aldehydes

EnvIRONmentally friendly: The title hydrogenation of aldehydes, ketones, and α,β-unsaturated aldehydes is reported. In the presence of the catalyst **1**, primary, secondary, and allylic alcohols were obtained in good to excellent yields under mild reaction conditions. The catalyst is easily and inexpensively prepared, and is also stable to air, water, and column chromatography.

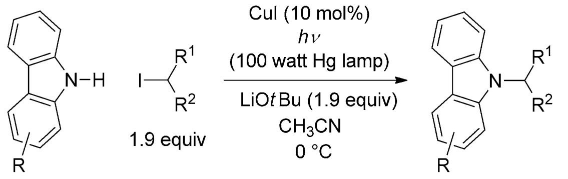


Synthetic Methods



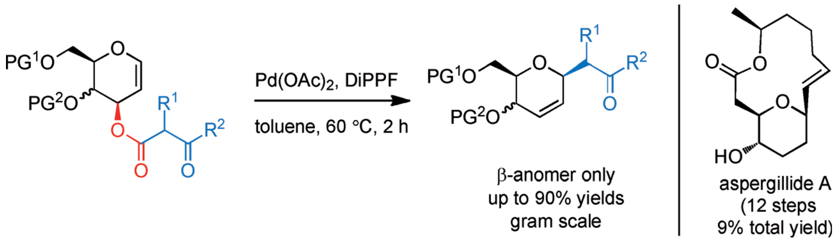
Friendly competition: A three-component reaction system composed of calcium carbide, an aryl aldehyde, and an amine gave enaminones or propargylamines (see picture) in a predictable manner through competitive pathways. The system enables the cost-efficient synthesis of a variety of enaminones from readily accessible small molecules and demonstrates the versatility of the acetylide ion, which can be used to bridge electrophiles and nucleophiles.

Homogeneous Catalysis



N-alkylations of carbazoles with a variety of secondary and hindered primary alkyl iodides can be achieved by using a simple precatalyst (CuI) under mild conditions (0 °C) in the presence of a Brønsted base; at higher temperature (30 °C), secondary alkyl bromides also serve as suitable coupling partners. A Li[Cu(carbazolide)$_2$] complex has been crystallographically characterized, and it may serve as an intermediate in the catalytic cycle.

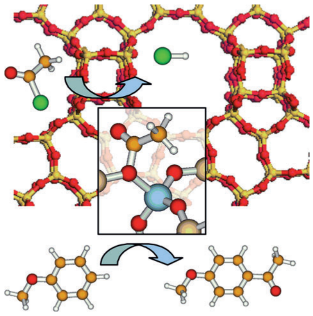
C-Glycosylation



Mild and sweet: The title reaction proceeds under mild conditions with high regio- and diastereoselectivity (see scheme, PG = protecting group, DiPPF = 1,1′-bis(diisopropylphosphino)ferrocene). This reaction is suitable for a wide range of glycal-derived γ-ketone esters and affords *C*-glycosides with exclusive β-selectivity. The method was further applied to a concise formal synthesis of aspergillide A.

Reaction Mechanisms

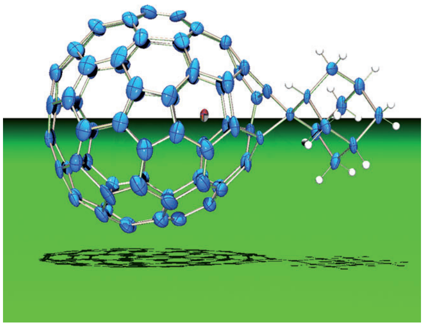
Finding the culprits: In situ NMR spectroscopy combined with theoretical calculations show the formation of acetyl species covalently bound to framework oxygen atoms in acid zeolites. These species, and not the usually assumed acylium cations, are the reactive intermediates in Friedel–Crafts acylation and Koch carbonylation reactions on zeolites.



Supramolecular Chemistry

Y. Xie, M. Suzuki, W. Cai, N. Mizorogi, S. Nagase, T. Akasaka,* X. Lu* ________________ **5142 – 5145**

Highly Regioselective Addition of Adamantylidene Carbene to Yb@C_{2v}(3)-C_{80} to Afford the First Derivative of Divalent Metallofullerenes

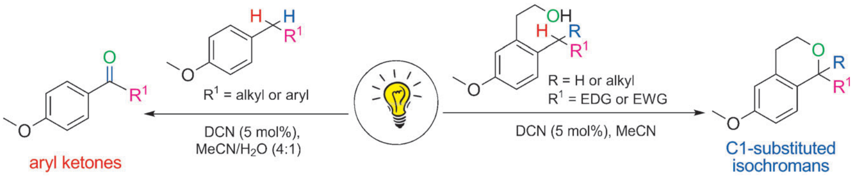


Divalent effect: The compound shown is the sole product in the cycloaddition reaction of adamantylidene carbene with Yb@C_{2v}(3)-C_{80}, and is the first derivative of a divalent metallofullerene. An unexpected strain-induced addition pattern and remarkable alterations of the metal position in response to exohedral modification are observed, thus illustrating there is an interplay between the divalent metal ion and the fullerene cage.

C–H Activation

G. Pandey,* S. Pal, R. Laha _ **5146 – 5149**

Direct Benzylic C–H Activation for C–O Bond Formation by Photoredox Catalysis



Power of light: 1,4-dicyanonaphthalene (DCN) and light directly activates benzylic C–H bonds for intra- and intermolecular C–O bond formation. Arylalkyls have also been transformed directly into aryl ketones using water as a source of oxygen. EDG = electron-donating group, EWG = electron-withdrawing group.

DOI: 10.1002/anie.201302562

50 Years Ago ...

Angewandte Chemie International Edition was first published in 1962, the mother journal first in 1888. In this monthly flashback, we feature some of the articles that appeared 50 years ago. This look back can open our eyes, stimulate discussion, or even raise a smile.

Fluorination was already popular 50 years ago, and two Communications on this topic were published in the same issue. P. Sartori discussed how the electrofluorination of gases that are insoluble in liquid HF could be achieved at atmospheric pressure by forcing the gases through the electrolyte from below. Propane, ethane, methane, and hydrogen sulfide were all electrofluorinated by using this procedure to give mixtures of products. Oskar Glemser, Herbert Roesky, and Karl-Heinz Hellberg reported the reaction of chromium powder with elemental fluorine at high temperature and pressure to produce chromium(V) fluoride and chromium(VI) fluoride as bright-red and lemon-yellow solids, respectively. The compositions of the solids were determined by analyzing the products resulting from hydrolysis. Roesky is in the top two authors who have published the most manuscripts in *Angewandte Chemie* from 1946–2012 (see the recent Review by François Diederich: *Angew. Chem. Int. Ed.* **2013**, *52*, 2714).

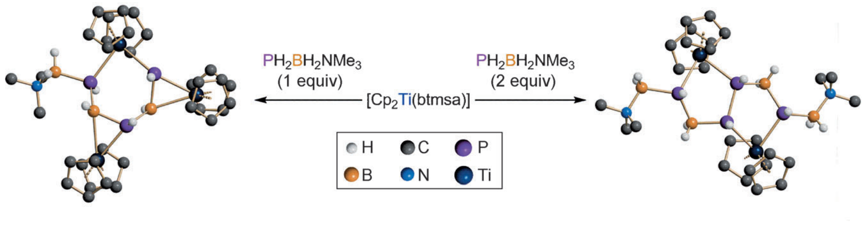
The Reviews section contained contributions by Herrmann Schmalzried on solid-state reactions between ionic crystals, including oxides, halides, and sulfides, and by Fritz Kröhnke on synthesis using pyridinium salts. The electronic properties of pyridinium cations make them ideal for use in a range of syntheses, including those of quinolizine rings, indole-3-carboxylic acids, and triarylpyrimidines.

Read more in Issue 5/1963

Phosphorus–Boron Oligomers

C. Thoms, C. Marquardt, A. Y. Timoshkin, M. Bodensteiner, M. Scheer* ———— 5150–5154

The Oligomerization of Phosphinoborane by Titanium Complexes

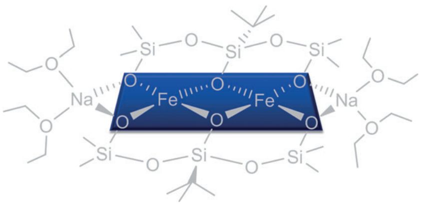


The PB chain gang: The reactions of an acetylene complex of titanocene with the parent phosphinoborane stabilized only by a Lewis base lead to novel phosphinoborane oligomers coordinated by $\{Cp_2Ti\}$ complex fragments. Depending on the reaction conditions (temperature and stoichiometry), unprecedented oligomeric chains of phosphinoborane are obtained by dehydro-oligomerization and P–P coupling reactions. btmsa = bis(trimethylsilyl)acetylene.

Coordination Chemistry

D. Pinkert, S. Demeshko, F. Schax, B. Braun, F. Meyer, C. Limberg* ———— 5155–5158

A Dinuclear Molecular Iron(II) Silicate with Two High-Spin Square-Planar FeO_4 Units



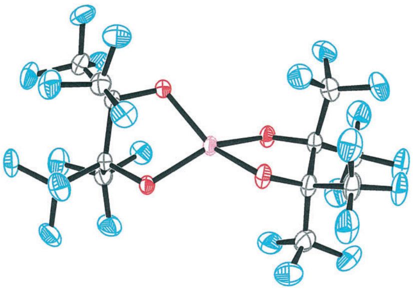
Ferrous flatland: Two flattened $Fe^{II}O_4$ units that share an edge are found in the title compound (see structure). They are spanned by tripodal silanolate ligands, which form in situ from a trisilanol if iron ions are available for complexation. The compound approaches the situation in the natural iron silicate gillespite or in certain ceramics where square planar FeO_4 units have also been found.

Coordination Chemistry

X. Wurzenberger, C. Neumann, P. Klüfers* ———— 5159–5161

Enticing Cobalt into Planarity: Can a Pair of Diolato Ligands Make It Happen?

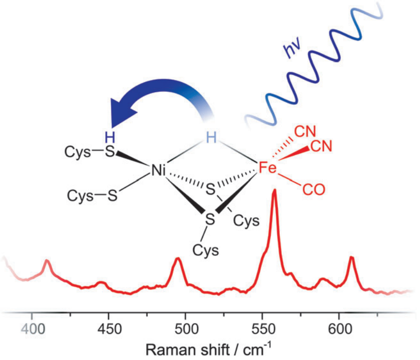
They can't do it alone: The Jahn–Teller instability found in the iron(II) species is missing in the homologous bis(perfluoropinacolato) cobalt(II) complex. Thus the stable conformation of the cobalt center is closer to tetrahedral than square planar, as shown by a DFT approach, and also in an isolatable salt (see structure).



Biocatalysis

E. Siebert, M. Horch,* Y. Rippers, J. Fritsch, S. Frielingsdorf, O. Lenz, F. Velazquez Escobar, F. Siebert, L. Paasche, U. Kuhlmann, F. Lendzian, M. A. Mroginski, I. Zebger,* P. Hildebrandt* ———— 5162–5165

Resonance Raman Spectroscopy as a Tool to Monitor the Active Site of Hydrogenases



Insights in active sites: Hydrogen-conversion by hydrogenase is mediated by a sophisticated, metal-containing catalytic center. Resonance Raman spectroscopy is used for the first time in the characterization of the active site of these biocatalysts. An integrated spectroscopic and computational approach gives insights into structural and photochemical properties of the active site of an oxygen-tolerant [NiFe] hydrogenase.

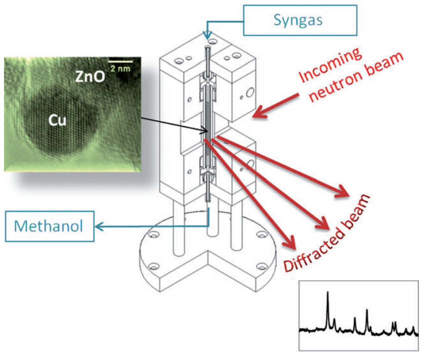
Back Cover

Heterogeneous Catalysis

T. Kandemir, F. Girgsdies, T. C. Hansen, K.-D. Liss, I. Kasatkin, E. L. Kunkes, G. Wowsnick, N. Jacobsen, R. Schlögl, M. Behrens* ______ **5166 – 5170**

In Situ Study of Catalytic Processes: Neutron Diffraction of a Methanol Synthesis Catalyst at Industrially Relevant Pressure

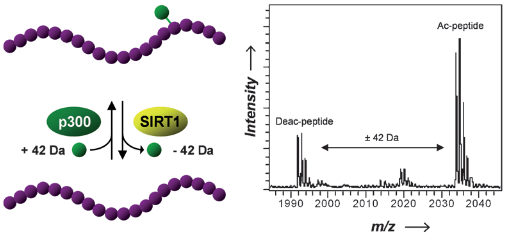
Studying the workplace: An industrial methanol synthesis catalyst operating at high pressure was studied by in situ neutron diffraction. The peculiar microstructure of Cu/ZnO/Al_2O_3 nanocatalysts was found to be stable under reaction conditions. Stacking fault annealing and brass formation was only observed at temperatures higher than used in the methanol synthesis process, providing support for active role of defects in this catalyst system.



Protein Mass Spectrometry

S. Holzhauser, A. Freiwald, C. Weise, G. Multhaup, C.-T. Han, S. Sauer* ______ **5171 – 5174**

Discovery and Characterization of Protein-Modifying Natural Products by MALDI Mass Spectrometry Reveal Potent SIRT1 and p300 Inhibitors

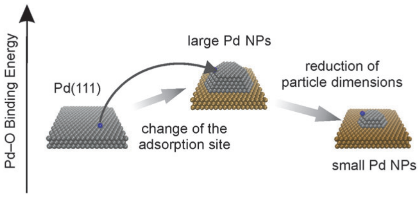


A straightforward MALDI MS method facilitates the unbiased screening and characterization of compounds that modify protein activity. This procedure can be used to circumvent analytical problems deriving from compounds with autofluorescence. Various posttranslationally active enzymes like deacetylases, acetyltransferases, kinases, phosphatases, and methyltransferases can be studied in the presented way.

Heterogeneous Catalysis

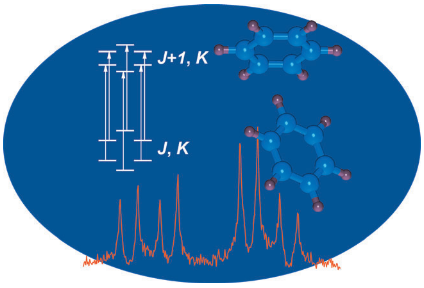
M. Peter, J. M. Flores Camacho, S. Adamovski, L. K. Ono, K.-H. Dostert, C. P. O'Brien, B. Roldan Cuenya, S. Schauermann,* H.-J. Freund ______ **5175 – 5179**

Trends in the Binding Strength of Surface Species on Nanoparticles: How Does the Adsorption Energy Scale with the Particle Size?



The binding energy of oxygen on Pd nanoparticles was measured by a direct calorimetric method as a function of the particle size. The reduced dimensionality of the Pd substrate results in two counteracting trends: an increase of the Pd–O binding strength due to a change of the local configuration of the adsorption site and a strong decrease of the Pd–O bonding due to the reduction of the cluster size.

The benzene dimer, an important prototype for studying noncovalent interactions, exhibits characteristic splitting patterns in its rotational spectrum, which for a long time were not understood. A new theoretical model reveals their origin: a concerted internal motion involving sixfold hindered rotation tunneling of the molecule forming the stem of the T-shaped structure and tilt tunneling of the cap.



Benzene Dimer

M. Schnell,* U. Erlekam, P. R. Bunker, G. von Helden, J.-U. Grabow, G. Meijer, A. van der Avoird* ________ **5180 – 5183**

Structure of the Benzene Dimer—Governed by Dynamics

Front Cover

Supporting information is available on www.angewandte.org (see article for access details).

A video clip is available as Supporting Information on www.angewandte.org (see article for access details).

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