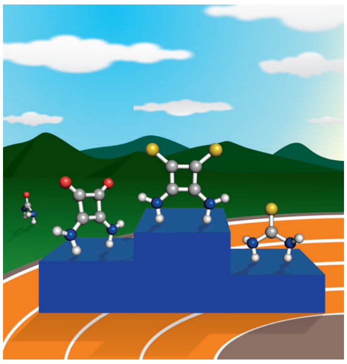
On these pages, we feature a selection of the excellent work that has recently been published in our sister journals. If you are reading these pages on a computer, click on any of the items to read the full article. Otherwise please see the DOIs for easy online access through Wiley Online Library.

Organocatalysis

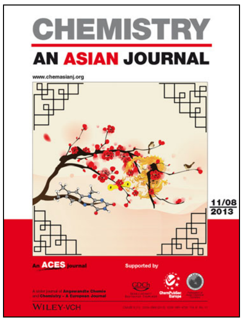
T. Lu, S. E. Wheeler*

Origin of the Superior Performance of (Thio)Squaramides over (Thio)Ureas in Organocatalysis

Bifunctional catalysts: The performance of (thio)squaramide and (thio)urea-derived aminocatalysts was probed computationally within the context of Diels–Alder cycloadditions of nitrostyrene and anthracene. A proposed thiosquaramide-based catalyst is predicted to give the lowest reaction barrier, which stems from the ability of thiosquaramides to engage in stronger hydrogen-bonding interactions.



Chem. Eur. J.
DOI: **10.1002/chem.201302990**

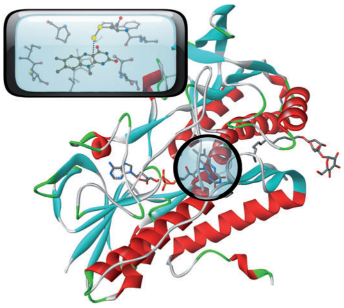


Enzymes

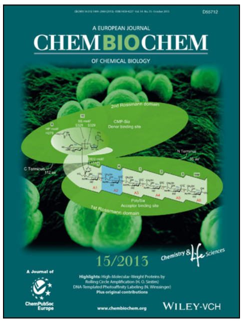
A. Bauzá, D. Quiñonero, P. M. Deyà, A. Frontera*

On the Importance of Anion–π Interactions in the Mechanism of Sulfide:Quinone Oxidoreductase

By a factor of FAD! Analysis of sulfide:quinone oxidoreductase (SQR; see picture) with and without the presence of flavin adenine dinucleotide (FAD) demonstrates the importance of anion–π interactions in the mechanism of action of sulfide oxidation. The nature of the addition–elimination mechanism has been analyzed and the barrier of the elimination step is reduced by the presence of the cofactor.



Chem. Asian J.
DOI: **10.1002/asia.201300786**

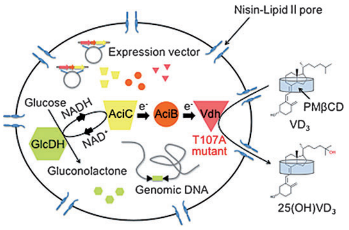


Biosynthesis

Y. Yasutake, T. Nishioka, N. Imoto, T. Tamura*

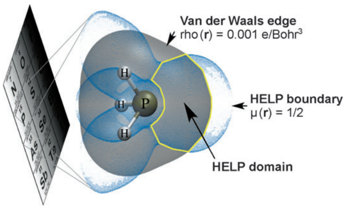
A Single Mutation at the Ferredoxin Binding Site of P450 Vdh Enables Efficient Biocatalytic Production of 25-Hydroxyvitamin D_3

Dramatic activity enhancement by a single mutation: A Highly active single mutant of P450 vitamin D_3 hydroxylase (Vdh) was obtained by engineering the ferredoxin-binding surface. Biocatalytic production of 25-hydroxyvitamin D_3 is reported, by using nisin-treated *Rhodococcus erythropolis* cells expressing the Vdh mutant.



ChemBioChem
DOI: **10.1002/cbic.201300386**

Lone Pairs

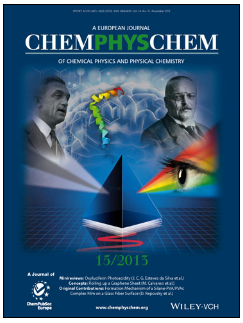


M. Rahm,* K. O. Christe

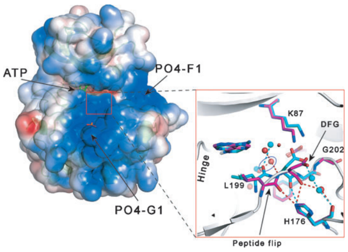
Quantifying the Nature of Lone Pair Domains

Help, HELP! The first chemically relevant quantification of the lone pair domain by quantum chemical topology calculations is demonstrated. A novel partitioning of the electron localization function is introduced. The complementarity of density- and orbital-based analyses of chemistry is discussed. This measure of the lone pair domain correlates well with a range of molecular and atomic properties, and is predicted to be of general use.

ChemPhysChem
DOI: **10.1002/cphc.201300723**



Drug Design



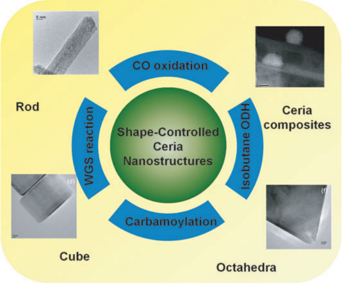
Y. Xue,* P. T. Wan, P. Hillertz, F. Schweikart, Y. Zhao, L. Wissler, N. Dekker*

X-ray Structural Analysis of Tau-Tubulin Kinase 1 and Its Interactions with Small Molecular Inhibitors

Flipped into place! The tau-tubulin kinase 1 (TTBK1) structure revealed two clear basic patches near the ATP pocket providing an explanation for phosphorylation-primed substrates. The structure in complex with compound **2** revealed a reorganization of the L199–D200 peptide backbone conformation together with altered hydrogen bonding. The analyses of TTBK1 binding to ligands with distinct characteristics could enable a fast track for structure-based ligand design of selective TTBK1 inhibitors.

ChemMedChem
DOI: **10.1002/cmdc.201300274**

Environmental Catalysis

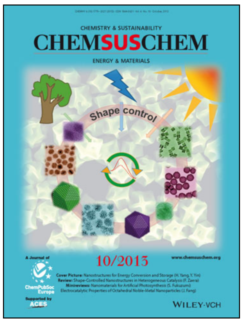


Z.-A. Qiao, Z. Wu,* S. Dai*

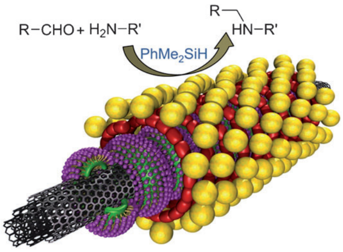
Shape-Controlled Ceria-based Nanostructures for Catalysis Applications

Ceria catalysis: The shape-controlled synthesis of ceria-based nanomaterials is of high importance for environment- and energy-related applications. This Minireview highlights the recent progress in the research of ceria nanoshapes as both catalysts and catalyst supports, including the synthesis, structure characterization, catalytic properties, surface chemistry, as well as reaction mechanism.

ChemSusChem
DOI: **10.1002/cssc.201300428**



Reductive Amination

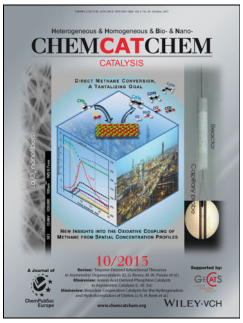


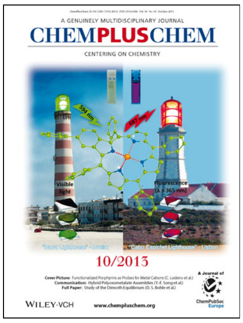
R. Kumar, E. Gravel, A. Hagège, H. Li, D. Verma, I. N. N. Namboothiri,* E. Doris*

Direct Reductive Amination of Aldehydes Catalyzed by Carbon Nanotube/Gold Nanohybrids

Gold digger: The direct reductive amination of aldehydes catalyzed by gold/carbon-nanotube nanohybrids with a silane as a hydride source is reported.

ChemCatChem
DOI: **10.1002/cctc.201300490**



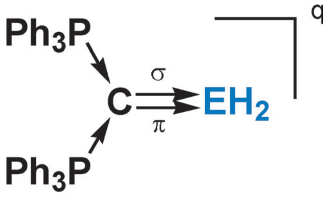


Bonding Analysis

M. A. Celik, G. Frenking,* B. Neumüller,* W. Petz*

Exploiting the Twofold Donor Ability of Carbodiphosphoranes: Theoretical Studies of $[(PPh_3)_2C\rightarrow EH_2]^q$ ($E^q = Be, B^+, C^{2+}, N^{3+}, O^{4+}$) and Synthesis of the Dication $[(Ph_3P)_2C{=}CH_2]^{2+}$

Give and take: Quantum chemical calculations of the carbodiphosphorane adducts $[(PPh_3)_2C\rightarrow EH_2]^q$ ($E^q = Be, B^+, C^{2+}, N^{3+}, O^{4+}$; see figure) give energy minima for $[(PPh_3)_2C\rightarrow BeH_2]$, $[(PPh_3)_2C\rightarrow BH_2]^+$, $[(PPh_3)_2C\rightarrow CH_2]^{2+}$, and $[(PPh_3)_2C\rightarrow NH_2]^{3+}$. Bonding analysis shows that $[(PPh_3)_2C\rightarrow BeH_2]$ and $[(PPh_3)_2C\rightarrow BH_2]^+$ possess donor–acceptor bonds, in which the σ and π lone-pair electrons of $(PPh_3)_2C$ donate into the vacant orbitals of the acceptor fragment.



E = Be, B, C, N, O

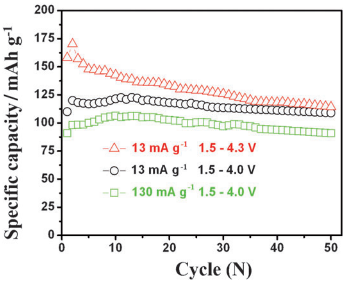
ChemPlusChem
DOI: **10.1002/cplu.201300169**

Sodium-Ion Batteries

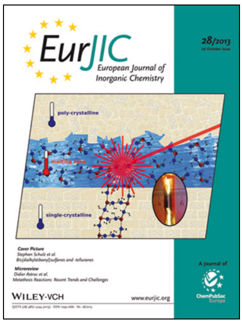
J. Xu, S.-L. Chou,* J.-L. Wang, H.-K. Liu, S.-X. Dou

Layered P2-$Na_{0.66}Fe_{0.5}Mn_{0.5}O_2$ Cathode Material for Rechargeable Sodium-Ion Batteries

Charging ahead: A layered P2-$Na_{0.66}Fe_{0.5}Mn_{0.5}O_2$ cathode material for use in sodium-ion batteries was synthesized by using the sol-gel method. The electrochemical performance results show that the as-prepared P2-$Na_{0.66}Fe_{0.5}Mn_{0.5}O_2$ electrode has a high energy density and good cycling performance.



ChemElectroChem
DOI: **10.1002/celc.201300026**

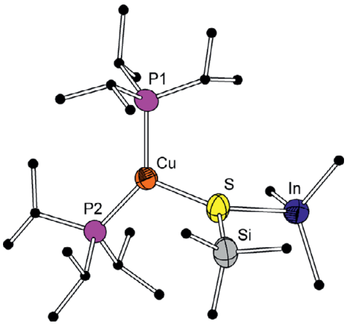


Lewis Acid–Base Adducts

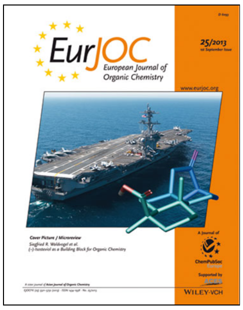
R. Biedermann, O. Kluge, D. Fuhrmann, H. Krautscheid*

Synthesis and Crystal Structures of $[(iPr_3P)_2Cu(\mu\text{-}ESiMe_3)(InMe_3)]$ (E = S, Se): Lewis Acid–Base Adducts with Chalcogen Atoms in Planar Coordination

Lewis acid–base adducts of trimethylindium and phosphane-stabilized copper(I) (trimethylsilyl)chalcogenolates were synthesized and characterized by X-ray crystal structure determination. They are very unstable under atmospheric conditions and decompose at ambient temperatures. DFT calculations reveal that the unusual planar coordination of the chalcogen atoms is due to steric crowding.



Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.201300768**

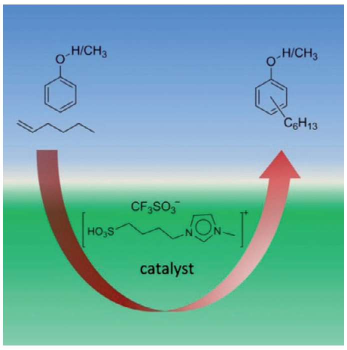


Ionic Liquids

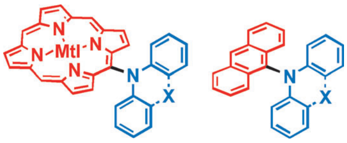
K. Titze-Frech, N. Ignatiev, M. Uerdingen, P. S. Schulz,*
P. Wasserscheid

Highly Selective Aromatic Alkylation of Phenol and Anisole by Using Recyclable Brønsted Acidic Ionic Liquid Systems

A sulfonic acid functionalized ionic liquid is used as catalyst in the hexylation of phenol and anisol, enabling very high product selectivities, simple product isolation and effective catalyst recycling. The observed selectivity boost is mainly due to differential solubility effects of the liquid–liquid biphasic reaction system established by the ionic liquid catalyst.



Eur. J. Org. Chem.
DOI: **10.1002/ejoc.201300579**



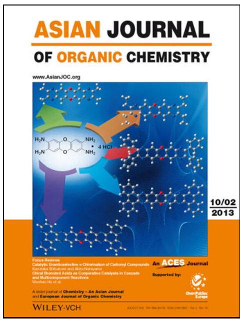
Porphyrin Amination

Y. Suzuki, N. Fukui, K. Murakami, H. Yorimitsu,* A. Osuka*

Amination of *meso*-Bromoporphyrins and 9-Haloanthracenes with Diarylamines Catalyzed by a Palladium–PEPPSI Complex

***meso* soup**: Palladium-catalyzed aminations of the bulky aryl halides *meso*-bromoporphyrins and 9-haloanthracenes with diarylamines provide efficient syntheses of *meso*-aminoporphyrins and 9-aminoanthracenes. Pd-PEPPSI complexes that have *N*-heterocyclic carbenes as ligands have the highest catalytic activities. The scope of diarylamines is wide enough to use diphenylamine, phenoxazine, phenothiazine, 9,10-dihydroacrydine, and carbazole.

Asian J. Org. Chem.
DOI: **10.1002/ajoc.201300162**



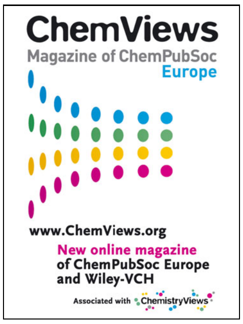
Sustainability

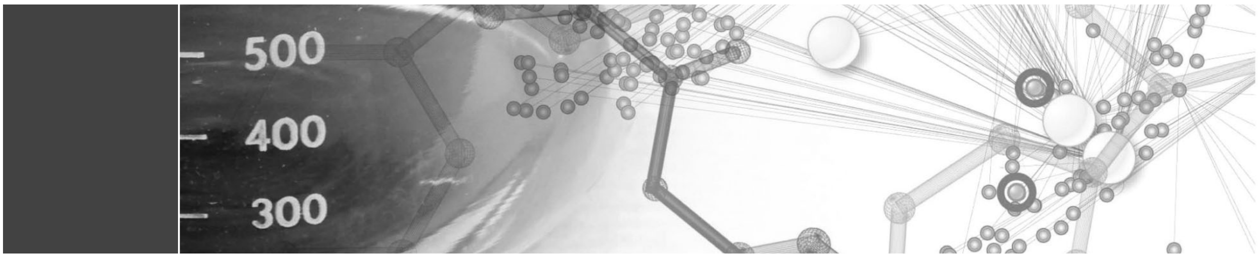
Sunil Herat

Environmentally Sound Management of E-Waste

With new designs and technology constantly being developed electrical and electronic equipment rapidly becomes obsolete. Thus, the environmentally safe disposal of this electronic waste (e-waste) is becoming an important issue, especially in developing countries. Sunil Herat, Griffith University, Australia, discusses various solutions to the issues associated with the management of this e-waste.

ChemViews magazine
DOI: **10.1002/chemv.201300101**





Novartis Chemistry Lectureship

Novartis is pleased to announce the following Novartis Chemistry Lecturers for 2013 – 2014.

Benjamin F. Cravatt
The Skaggs Institute for Chemical Biology
The Scripps Research Institute
La Jolla, CA, USA

Robert Glen
University of Cambridge
Cambridge, UK

Kenichiro Itami
Nagoya University
Nagoya, Japan

Andreas Kirschning
Leibniz University of Hannover
Hannover, Germany

Gary A. Molander
University of Pennsylvania
Philadelphia, PA, USA

Christopher D. Vanderwal
University of California at Irvine
Irvine, CA, USA

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The Novartis Chemistry Lectureship is awarded to scientists in recognition of outstanding contributions to organic and computational chemistry, including applications to biology.