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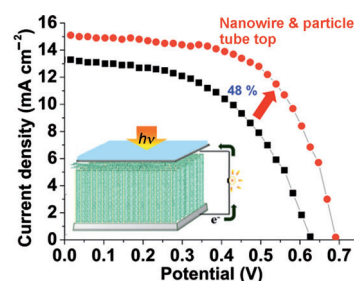


Nanostructures

N. Mir, K. Lee, I. Paramasivam, P. Schmuki*

Optimizing TiO₂ Nanotube Top Geometry for Use in Dye-Sensitized Solar Cells

Recombination dynamics: For TiO₂ nanotube-based dye-sensitized solar cells, the efficiency can be drastically enhanced by a synergetic effect that occurs when using nanowire-ended nanotubes in combination with an adequate nanoparticle decoration (see figure).



Chem. Eur. J.
DOI: 10.1002/chem.201202002

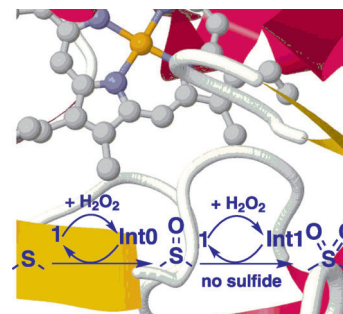


Bioinorganic Chemistry

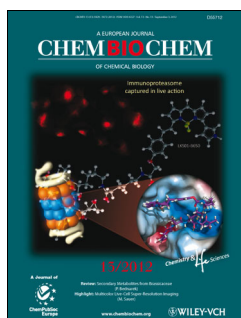
X. Zhou,* X. Chen, Y. Jin, I. E. Markó*

Evidence of Two Key Intermediates Contributing to the Selectivity of P450-Biomimetic Oxidation of Sulfides to Sulfoxides and Sulfones

A mild process for the selective oxidation of sulfides is in great demand. Therefore, probing the mechanism underlying the biological oxidation of sulfides under ambient conditions may provide valuable insights for the development of such a reaction. Based on porphyrin models of P450 enzymes, evidence of two key intermediates, **Int0** and **Int1**, in this reaction is provided.



Chem. Asian J.
DOI: 10.1002/asia.201200422

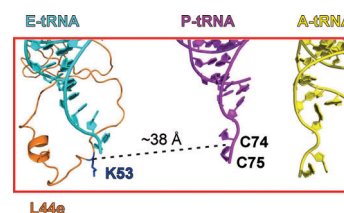


Transfer RNA

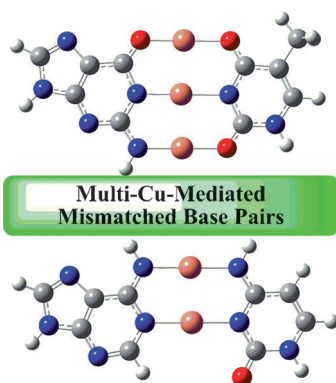
C. Hountondji,* K. Bulygin, A. Woisard, P. Tuffery, J.-B. Cr chet, M. Pech, K. H. Nierhaus, G. Karpova, S. Baouz

Lys53 of Ribosomal Protein L36AL and the CCA End of a tRNA at the P/E Hybrid Site Are in Close Proximity on the Human Ribosome

RNA–protein interactions: C74/75 of a P/E tRNA can be crosslinked to K53 of L44e, the only protein adjacent to the CCA end of a ribosomal bound tRNA. L44e has remarkable features: for example, a universally conserved GGQ motif—the Q residue—contains one of seven identified modifications, thus suggesting that this protein might be a preferential target for regulation.



ChemBioChem
DOI: 10.1002/cbic.201200208

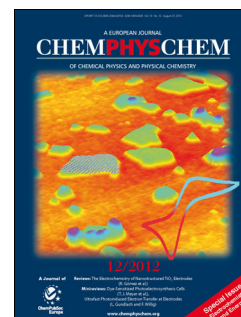


Nanowires

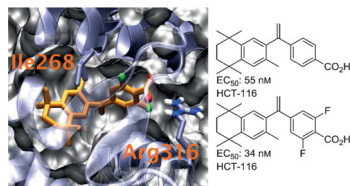
J. Zhao, L. Han, H. Yang, J. Liu, Y. Bu*

Rational Design for Building Blocks of DNA-Based Conductive Nanowires through Multi-Copper Incorporation into Mismatched Base Pairs

Introduction of short copper chains into mismatched DNA base pairs (GT and AC, see picture) leads to two multi-Cu-mediated base pairs that have different electronic properties from those of the natural base pairs and the multi-Zn-mediated natural ones. This work provides an executable strategy to yield DNA building blocks with adjustable properties for DNA-based molecular wire and electronic devices.



ChemPhysChem
DOI: 10.1002/cphc.201200419

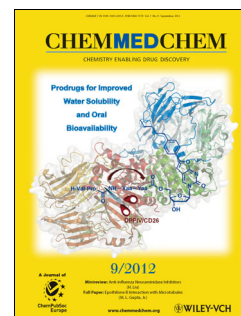


Anticancer Agents

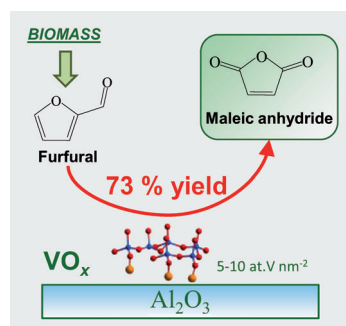
J. K. Furmick, I. Kaneko, A. N. Walsh, J. Yang, J. S. Bhogal, G. M. Gray, J. C. Baso, D. O. Browder, J. L. S. Prentice, L. A. Montano, C. C. Huynh, L. M. Marcus, D. G. Tsosie, J. S. Kwon, A. Quezada, N. M. Reyes, B. Lemming, P. Saini, A. van der Vaart, T. L. Groy, P. A. Marshall, P. W. Jurutka, C. E. Wagner*

Modeling, Synthesis and Biological Evaluation of Potential Retinoid X Receptor-Selective Agonists: Novel Halogenated Analogues of 4-[1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydro-2-naphthyl)ethynyl]benzoic Acid (Bexarotene)

Transcriptional signaling: An analogue of bexarotene with two fluorine atoms *ortho* to the carboxylic acid group has a lower EC₅₀ value (34 nm) than bexarotene (55 nm) for the retinoid X receptor in HCT-116 cells. A low-energy docked conformation of the difluorobexarotene analogue in the ligand binding pocket of RXR as modeled in AutoDock 4.2 is shown.



ChemMedChem
DOI: 10.1002/cmdc.201200319

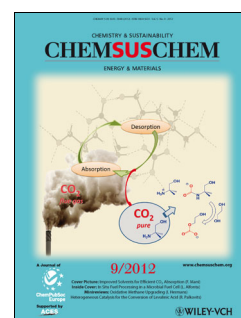


Biorefineries

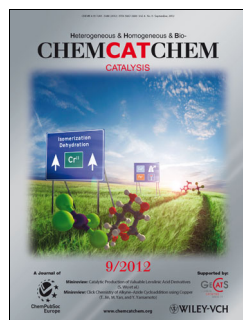
N. Alonso-Fagúndez, M. L. Granados, R. Mariscal, M. Ojeda*

Selective Conversion of Furfural to Maleic Anhydride and Furan with VO_x/Al₂O₃ Catalysts

Toward future biorefineries: We demonstrate here a promising route to convert renewable furfural to maleic anhydride (max. 73 % yield) and furan (max. 9% yield) through selective gas-phase oxidation with O₂ by using VO_x/Al₂O₃ (0–25 at_v nm⁻²) as solid catalysts. This alternative catalytic technology allows the use of biomass instead of petroleum to synthesize these important chemicals for industry.



ChemSusChem
DOI: 10.1002/cssc.201200167

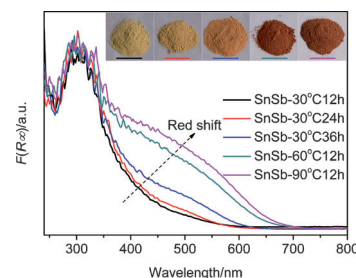


Photocatalysis

J. Shi, L. Ma, P. Wu, Z. Zhou, J. Jiang, X. Wan, D. Jing, L. Guo*

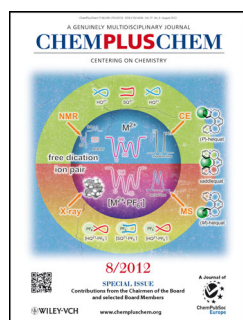
Tin(II) Antimonates with Adjustable Compositions: Effects of Band-Gaps and Nanostructures on Visible-Light-Driven Photocatalytic H₂ Evolution

Everlas-tin love: A series of tin(II) antimonates with varied Sn content were found to be stable and efficient photocatalysts for visible-light-driven H₂-evolution. Moreover, the relationships between their physicochemical properties—in particular their band-gaps (see figure) and nanostructures—and their photocatalytic activities were comprehensively investigated.



ChemCatChem

DOI: 10.1002/cctc.201200063

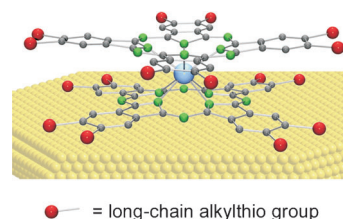


Single-Molecule Magnets

U. Glebe, T. Weidner, J. E. Baio, D. Schach, C. Bruhn, A. Buchholz, W. Plass, S. Walleck, T. Glaser, U. Siemeling*

Self-Assembled Monolayers of Single-Molecule Magnets [Tb{Pc'(SR)₈}₂] on Gold

SMM SAMs: The magnetic properties of bis(phthalocyaninato)terbium(III) complexes [Tb{Pc'(SR)₈}₂] bearing eight peripheral alkylthio substituents SR (R = n-C₈H₁₇, n-C₁₂H₂₅; see figure) were studied by SQUID measurements. These highly soluble single-molecule magnets were self-assembled from solution onto solid gold substrates and the self-assembled monolayers characterised by XPS, NEXAFS and AFM measurements.



ChemPlusChem

DOI: 10.1002/cplu.201200043

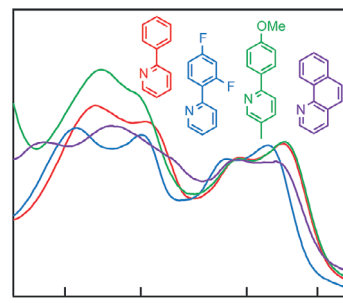


Coordination Compounds

M. L. Muro-Small, J. E. Yarnell, C. E. McCusker, F. N. Castellano*

Spectroscopy and Photophysics in Cyclometalated Ru^{II}-Bis(bipyridyl) Complexes

Cyclometalated Ru^{II} coordination compounds of the general formula [Ru(bpy)₂ΛN]PF₆ {CΛN = 2-phenylpyridine (1), 2-(2,4-difluorophenyl)pyridine (2), 2-(4-methoxyphenyl)-5-methylpyridine (3), benzo[h]quinoline (4); bpy = 2,2'-bipyridine} have been synthesized, structurally and electrochemically characterized, and examined with spectroscopic techniques including ultrafast transient absorption.



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201200460

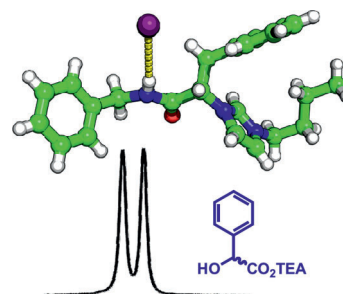


Ionic Liquids

L. González, B. Altava,* M. Bolte, M. I. Burguete, E. García-Verdugo, S. V. Luis*

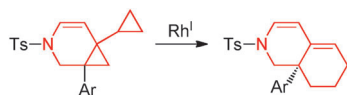
Synthesis of Chiral Room Temperature Ionic Liquids from Amino Acids – Application in Chiral Molecular Recognition

New chiral room temperature ionic liquids, based on an imidazolium group and derived from natural amino acids, have been synthesized and studied as chiral shift agents for the chiral discrimination of enantiomeric carboxylate salts.



Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201200607



Metal-Catalyzed Rearrangements

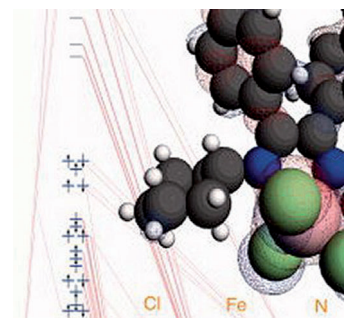
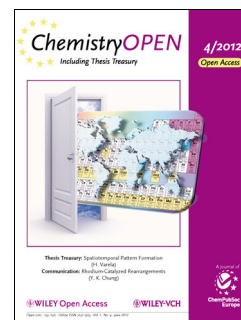
S. Son, S. Y. Kim, Y. K. Chung*

Rhodium-Catalyzed Rearrangement Reaction of Azabicyclo[4.1.0]heptenes bearing Cyclopropyl and Aryl Groups to Arylhexahydroisoquinolines

Let's rearrange! Rh(PPh₃)₂(CO)Cl/AgBF₄ has been found to be an efficient catalytic system in the rearrangement of azabicyclo[4.1.0]heptenes having an aryl and a cyclopropyl group in the 1- and 6-position, respectively. This has led to the development of an efficient and simple method for the synthesis of arylhexahydroisoquinolines.

ChemistryOpen

DOI: 10.1002/open.201200022



ChemViews magazine

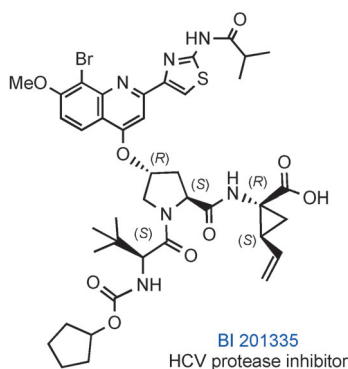
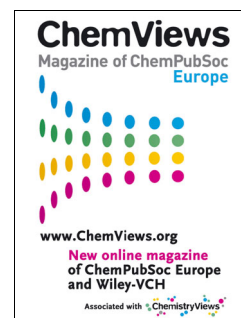
DOI: 10.1002/chemv.201200080

Spin-state Splittings

Madhusudan Singh and Matteo Cavalleri

The Challenges of Accounting for Spin-States of Molecules

Spin, a fundamental property of atoms and molecules, greatly impacts numerous physio-chemical phenomena in enzymatic synthesis, spin-crossover compounds, metal-oxo complexes, and catalysis. The difficulty of modeling spin states is reviewed with particular attention given to two applications with far-reaching consequences: metal-oxo complexes and spin-crossover compounds.



Asian J. Org. Chem.

DOI: 10.1002/ajoc.201200014

Synthetic Methods

C. A. Busacca,* X. Wei,* N. Haddad, S. Kapadia, J. C. Lorenz, A. K. Saha, R. J. Varsolona, T. Berkenbusch, S. C. Campbell, V. Farina, X. Feng, N. C. Gonnella, N. Grinberg, P.-J. Jones, H. Lee, Z. Li, O. Niemeier, W. Samstag, M. Sarvestani, J. Schroeder, J. Smoliga, E. M. Spinelli, J. Vitous, C. H. Senanayake

Practical Large-Scale Synthesis of the Hepatitis C Virus Protease Inhibitor BI 201335

Upsizing: A large-scale synthesis of BI 201335, which is a new drug for the treatment of hepatitis C infection, is described. BI 201335 has a molecular weight of 870, six rings, and five stereocenters. The synthetic route has high convergence, with a late-stage S_NAr reaction between a heterocyclic sulfone and a dipeptide acid. All of the peptide couplings were performed without protecting groups or hazardous reagents and without measurable racemization.

