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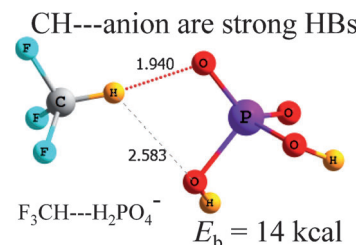


### Quantum Chemical Calculations

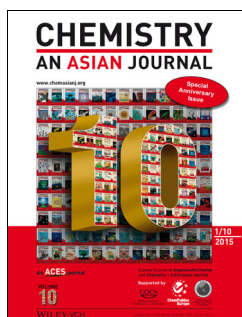
B. Nepal, S. Scheiner\*

Anionic  $\text{CH}\cdots\text{X}^-$  Hydrogen Bonds: Origin of Their Strength, Geometry, and Other Properties

**$\text{CF}_3\text{H}$  as a proton donor** was paired with a variety of anions, and its properties were assessed by MP2/aug-cc-pVDZ calculations (see figure). The binding energy of monoanions halide,  $\text{NO}_3^-$ , formate, acetate,  $\text{HSO}_4^-$ , and  $\text{H}_2\text{PO}_4^-$  lie in the 12–17 kcal mol $^{-1}$  range. Dianions  $\text{SO}_4^{2-}$  and  $\text{HPO}_4^{2-}$  are bound by 27 kcal mol $^{-1}$ , and trianion  $\text{PO}_4^{3-}$  by 45 kcal mol $^{-1}$ .



Chem. Eur. J.  
DOI: 10.1002/chem.201404970

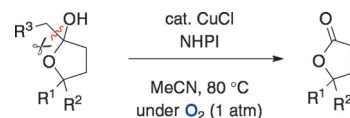


### Copper Catalysis

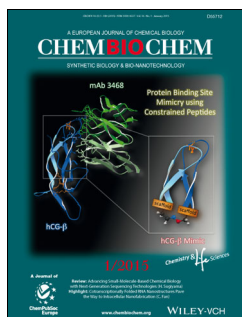
Y. L. Tnay, S. Chiba\*

Copper-Catalyzed Aerobic C–C Bond Cleavage of Lactols with N-Hydroxy Phthalimide for Synthesis of Lactones

**Let's get physical:** A Cu-catalyzed aerobic C–C bond cleavage of cyclic hemiacetals (lactols) into lactones was achieved in the presence of N-hydroxy phthalimide (NHPI). This reaction is composed of a multistep sequence including a) formation of *exo*-cyclic enol ethers through dehydration; b) addition of phthalimide N-oxyl radical to the enol ethers followed by trap of the resulting C-radicals with molecular oxygen to form peroxy radicals; c) reductive generation of oxy radicals and subsequent  $\beta$ -radical fragmentation to generate lactones.



Chem. Asian J.  
DOI: 10.1002/asia.201403196

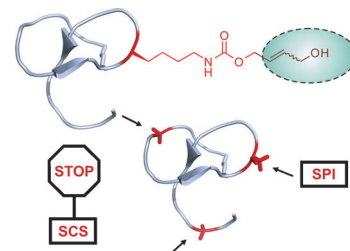


### Cyclic Peptides

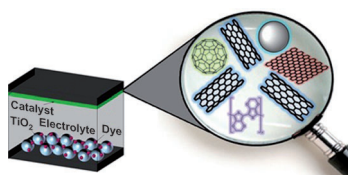
R. S. Al Toma, A. Kuthning, M. P. Exner, A. Denisiuk, J. Ziegler, N. Budisa, R. D. Süssmuth\*

Site-Directed and Global Incorporation of Orthogonal and Isostructural Noncanonical Amino Acids into the Ribosomal Lasso Peptide Capistrucin

**Expansion of the peptidic code:** Supplementation-based incorporation (SPI) and stop-codon suppression (SCS) approaches were used for co-translational incorporation of noncanonical amino acids into the lasso peptide, capistrucin. This use of synthetic biology gives a new way to produce lasso peptides *in vivo* starting from a wide range of amino acids.



ChemBioChem  
DOI: 10.1002/cbic.201402558



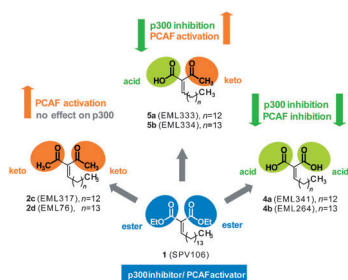
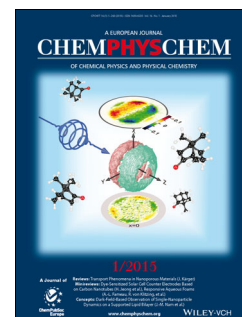
ChemPhysChem  
DOI: 10.1002/cphc.201402570

## Solar Cells

S. Hwang, M. Batmunkh, M. J. Nine, H. Chung, H. Jeong\*

Dye-Sensitized Solar Cell Counter Electrodes Based on Carbon Nanotubes

**Counter strike:** Platinum-based counter electrodes and the application of carbon nanotubes (CNTs) and their derivatives as promising alternatives to this precious platinum cathode in dye-sensitized solar cells are reviewed. On the basis of recent advances, promising research directions for the future accomplishment of CNT-based materials in this context are presented.



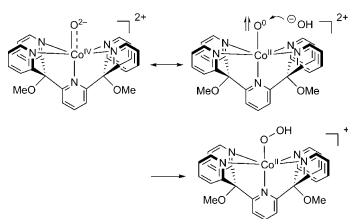
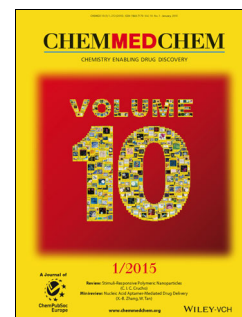
ChemMedChem  
DOI: 10.1002/cmdc.201402371

## Epigenetics

S. Castellano, C. Milite, A. Feoli, M. Viviano, A. Mai, E. Novellino, A. Tosco,\* G. Sbardella\*

Identification of Structural Features of 2-Alkylidene-1,3-Dicarbonyl Derivatives that Induce Inhibition and/or Activation of Histone Acetyltransferases KAT3B/p300 and KAT2B/PCAF

**Ups and downs:** Chemical manipulation of the carbonyl functional groups of a series of analogues of diethyl pentadecylenemalonate **1** (SPV106), a mixed inhibitor/activator of lysine acetyltransferases that we recently identified, yielded different activity profiles against KAT2B and KAT3B (pure KAT2B activator, pan-inhibitor, or mixed KAT2B activator/KAT3B inhibitor).



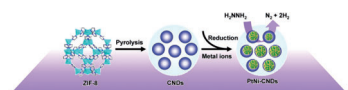
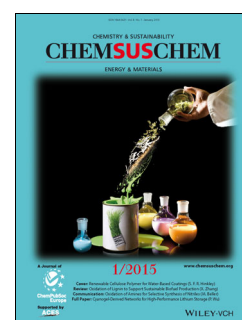
ChemSusChem  
DOI: 10.1002/cssc.201403024

## Water Oxidation

D. W. Crandell, S. Ghosh, C. P. Berlinguette,\* M.-H. Baik\*

How a  $[\text{Co}^{\text{IV}}=\text{O}]^{2+}$  Fragment Oxidizes Water: Involvement of a Biradicaloid  $[\text{Co}^{\text{II}}-(\cdot\text{O})]^{2+}$  Species in Forming the O–O Bond

**Quantum leap:** Quantum chemical models based on density functional theory are used to study the mechanism of water oxidation performed by a recently discovered cobalt complex (Py5 = 2,6-bis(bis-2-pyridyl)-methoxymethane)pyridine). It was shown that the most catalytically active species is the intermediate-spin quartet complex that is almost isoenergetic with the doublet state.



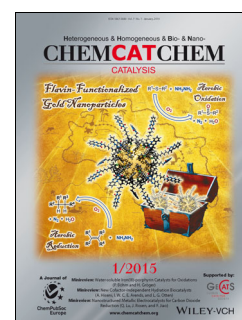
ChemCatChem  
DOI: 10.1002/cctc.201402735

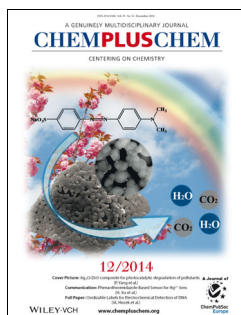
## Carbon Nanodots

J.-K. Sun, Q. Xu\*

Metal Nanoparticles Immobilized on Carbon Nanodots as Highly Active Catalysts for Hydrogen Generation from Hydrazine in Aqueous Solution

**Dot dot dot:** Highly dispersed bimetallic PtNi nanoparticles with different PtNi compositions have been immobilized on ZIF-8-derived carbon nanodots (CNDs). These materials show high catalytic activity and durability for hydrogen generation from the decomposition of hydrazine in aqueous solution at room temperature.



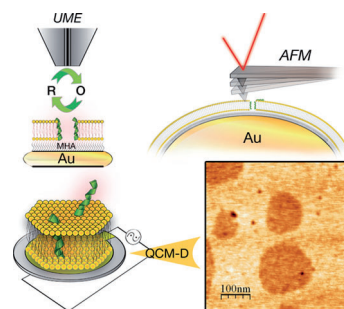


## Peptides

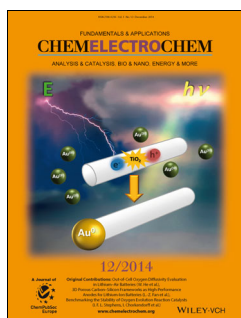
S. Piantavigna, M. E. Abdelhamid, C. Zhao, X. Qu, G. A. McCubbin, B. Graham, L. Spiccia, A. P. O'Mullane,\* L. L. Martin\*

Mechanistic Details of the Membrane Perforation and Passive Translocation of TAT Peptides

**The worm turns:** How does the TAT peptide translocate across a mammalian cell membrane? Three biophysical methods, which can spatially resolve scales from millimeter (quartz crystal microbalance with dissipation (QCM-D)) and micrometer (scanning electrochemical microscopy (SECM)) to nanometer (AFM), provide evidence for worm-hole-like pores (see figure). The SECM image shows that these pores allow redox mediators to pass through to the sensor, but TAT disrupts bacterial-mimetic membranes.



ChemPlusChem  
DOI: 10.1002/cplu.201402209

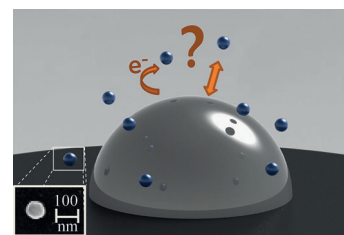


## Electrostatic Interactions

K. Tschulik, W. Cheng, C. Batchelor-McAuley, S. Murphy, D. Omanović, R. G. Compton\*

Non-Invasive Probing of Nanoparticle Electrostatics

**Not what you might think:** A new and non-invasive technique to probe the electrostatic interaction between surface-charged nanoparticles and a charged metal/solution interface shows that electrostatic effects are insignificant in all but very dilute electrolytes.



ChemElectroChem  
DOI: 10.1002/celc.201402285

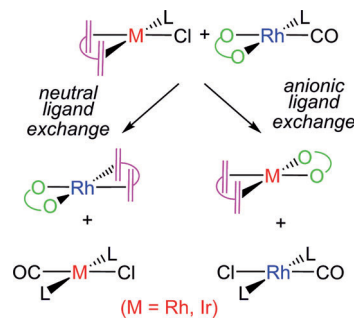


## Rhodium(I) Ligand Exchange

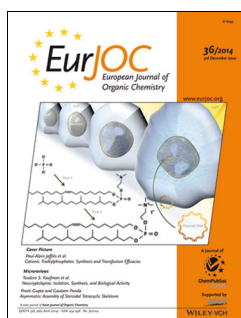
S. Chen, E. Manoury, R. Poli\*

Slow Exchange of Bidentate Ligands between Rhodium(I) Complexes: Evidence of Both Neutral and Anionic Ligand Exchange

Complexes [Rh(acac)(CO)(L<sup>1</sup>)] and [RhCl(COD)(L<sup>2</sup>)] undergo a very rapid double exchange of the monodentate phosphine ligands followed by a much slower exchange process involving the bidentate ligands.



Eur. J. Inorg. Chem.  
DOI: 10.1002/ejic.201402810

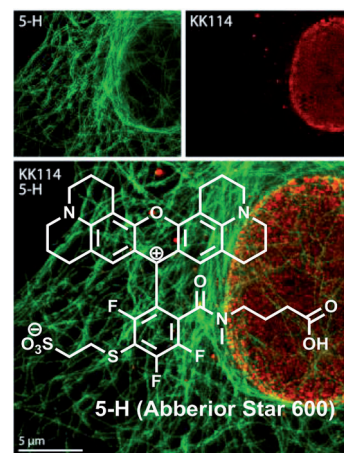


## Dyes for Microscopy

G. Yu. Mitronova,\* S. Polyakova, C. A. Wurm, K. Kolmakov, T. Wolfram, D. N. H. Meineke, V. N. Belov,\* M. John,\* S. W. Hell

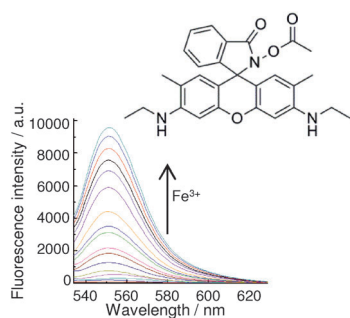
Functionalization of the *meso*-Phenyl Ring of Rhodamine Dyes Through S<sub>N</sub>Ar with Sulfur Nucleophiles: Synthesis, Biophysical Characterizations, and Comprehensive NMR Analysis

Aromatic nucleophilic substitution of fluorine in 9-(3'-carboxy-4',5',6',7'-trifluorophenyl) groups of xanthene dyes is regioselective (for thiols and amines). The reaction was used for the synthesis of a "bright" and very photostable dye for two-color superresolution microscopy. Characteristics of the NMR spectra may be used for structure elucidation of other fluorescent dyes.



Eur. J. Org. Chem.  
DOI: 10.1002/ejoc.201403269





ChemistryOpen

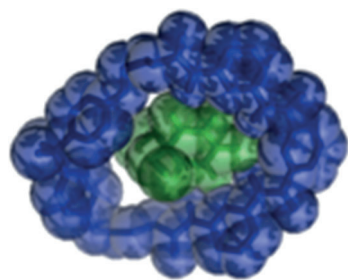
DOI: 10.1002/open.201402065

### Molecular Sensors

Z.-Q. Hu,\* Y.-Y. Gu, W.-Z. Hu, L.-L. Sun, J.-H. Zhu, Y. Jiang\*

A Highly Selective and Sensitive Turn-On Fluorescent Chemosensor Based on Rhodamine 6G for Iron(III)

**Iron you glad to see me:** Herein, we report an easily synthesized turn-on fluorescent  $\text{Fe}^{3+}$  chemosensor based on rhodamine. The sensor displays highly selective and sensitive  $\text{Fe}^{3+}$ -amplified fluorescence emission in acetonitrile even in the presence of other commonly interfering metal ions. Such fluorescent sensors for  $\text{Fe}^{3+}$  attract much attention due to the importance of  $\text{Fe}^{3+}$  in biological processes.



Asian J. Org. Chem.

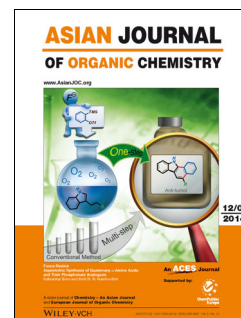
DOI: 10.1002/ajoc.201402243

### Barbiturate Receptors

A. Tron, M. Rocher, P. J. Thornton, J. H. R. Tucker,\*  
N. D. McClenaghan\*

Supramolecular Architectures Incorporating Hydrogen-Bonding Barbiturate Receptors

**Good hosts:** An overview of Hamilton-type bis(amidopyridine) receptor motifs, which offer strong and selective binding in non-competitive media for barbiturates and cyanurates, leading to a wide range of supramolecular assemblies, is presented. A particular emphasis is placed on photoaddressable systems.



ChemViews magazine

DOI: 10.1002/chemv.201400121

### Career

V. Köster

Career: As a Chemist at a Chemical Society

In an interview series, *ChemistryViews.org* gives readers a glimpse into the wide range of career paths in chemistry. This time, Dr. Karin J. Schmitz, head of career services at GDCh (German Chemical Society), talks about why she chose working at a chemical society over the lab and which skills are important to support chemists in various aspects of their professional life.

