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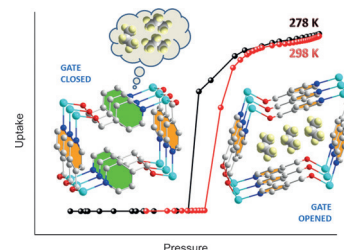


Coordination Chemistry

D. Banerjee, H. Wang, A. M. Plonka, T. J. Emge, J. B. Parise, J. Li*

Direct Structural Identification of Gas Induced Gate-Opening Coupled with Commensurate Adsorption in a Microporous Metal–Organic Framework

Gate crashing: The gate-opening mechanism of a microporous metal–organic framework was investigated. The gate-opening was found to occur though the rotation of organic rings in the presence of specific adsorbates. The energy diagram of gate-opening is also discussed.



Chem. Eur. J.
DOI: [10.1002/chem.201601784](https://doi.org/10.1002/chem.201601784)

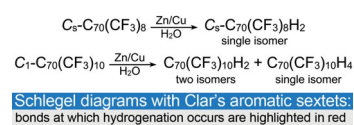


Fullerenes

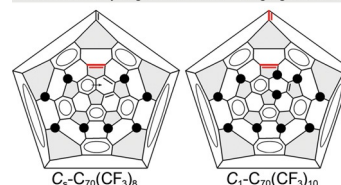
V. A. Brotsman, V. P. Bogdanov, A. V. Rybalchenko, E. P. Galanicheva, N. M. Belov, V. Y. Markov, N. S. Lukonina, I. N. Ioffe, S. I. Troyanov, E. Kemnitz, A. A. Goryunkov*

Reductive Hydrogenation of $C_5-C_{70}(CF_3)_8$ and $C_1-C_{70}(CF_3)_{10}$

CF_3 -derivatized fullerenes prove once again to be promising scaffolds for regioselective fullerene functionalization: now with the smallest possible addends—hydrogen atoms. The observed selectivity is governed by the electronic structure of the trifluoromethylated substrates. Interestingly, we discovered that Clar's theory can be utilized to predict the regiochemistry of functionalization.



Schlegel diagrams with Clar's aromatic sextets: bonds at which hydrogenation occurs are highlighted in red



Chem. Asian J.
DOI: [10.1002/asia.201600491](https://doi.org/10.1002/asia.201600491)

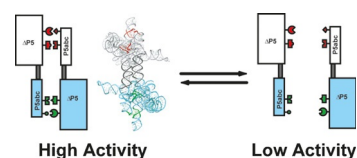


Ribozymes

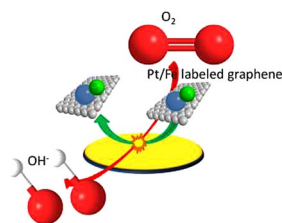
T. Tanaka, S. Matsumura, H. Furuta, Y. Ikawa*

Tecto-GIRz: Engineered Group I Ribozyme the Catalytic Ability of Which Can Be Controlled by Self-Dimerization

Tecto group I ribozyme: Dimeric RNA structures were designed based on the *Tetrahymena* group I ribozyme. These exhibited catalytic ability depending on controlled dimerization. Modular redesign of large ribozymes provides novel modular parts for RNA nanotechnology and RNA synthetic biology.



ChemBioChem
DOI: [10.1002/cbic.201600190](https://doi.org/10.1002/cbic.201600190)



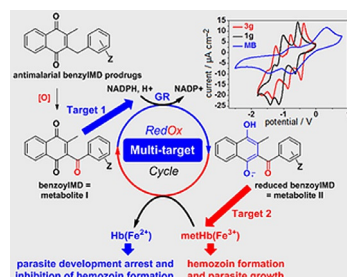
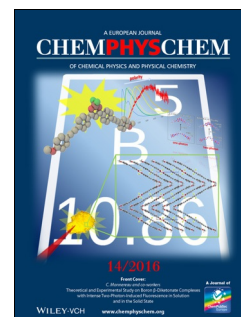
ChemPhysChem
DOI: 10.1002/cphc.201600237

Graphene

R. A. Thearle, Z. Sofer, D. Bouša, M. Pumera*

Impact Electrochemistry: Detection of Graphene Nanosheets Labeled with Metal Nanoparticles through Oxygen Reduction Mediation

Crash course: Graphene sheets can be detected upon impact at the electrode surface when they are labeled with catalytic Fe/Pt or Fe nanoparticles by using an indirect detection mode. Upon impact, these Fe/Pt- or Fe-labeled graphene sheets catalyze oxygen reduction, which leads to a significant reduction in current (see picture).



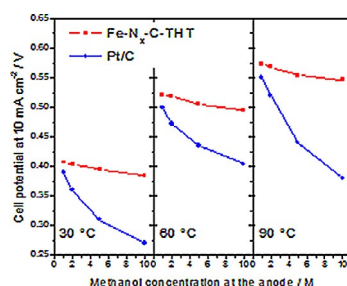
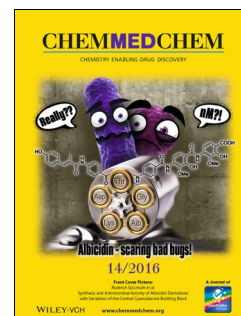
ChemMedChem
DOI: 10.1002/cmdc.201600009

Redox Polypharmacology

P. Sidorov, I. Desta, M. Chessé, D. Horvath, G. Marcou, A. Varnek, E. Davioud-Charvet,* M. Elhabiri*

Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites

Revisiting redox: Redox cyclers were quantified at the electrochemical level and modeled using QSPR predictive tools built in house for a series of 3-benzylmenadiones and their corresponding 3-benzoylmenadione redox-active metabolites. Drug bioactivation by benzylic oxidation was observed to be crucial and is correlated with the multitarget mechanism of action against *Plasmodium* spp. involving glutathione reductase and ferric species of hemoglobin.



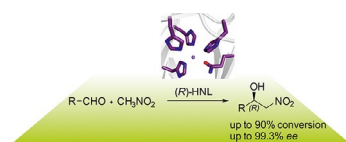
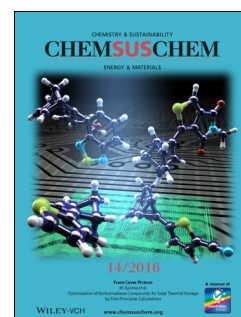
ChemSusChem
DOI: 10.1002/cssc.201600583

Fuel Cells

D. Sebastián, A. Serov, K. Artyushkova, J. Gordon, P. Atanasov,* A. S. Aricò, V. Baglio*

High Performance and Cost-Effective Direct Methanol Fuel Cells: Fe-N-C Methanol-Tolerant Oxygen Reduction Reaction Catalysts

No nobles here! Platinum group metal-free materials based on Fe-N-C are investigated as cost-effective, active, stable and methanol-tolerant catalysts for the oxygen reduction reaction (ORR) in direct methanol fuel cells (DMFCs). Outstanding performance of DMFCs is observed, even at high methanol concentration (10 M), owing to improved ORR activity and high tolerance to the alcohol.



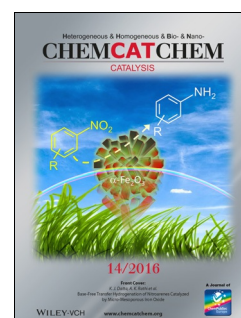
ChemCatChem
DOI: 10.1002/cctc.201600150

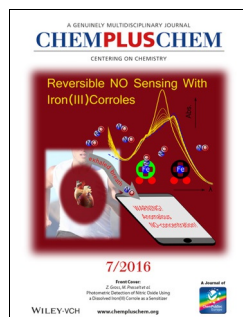
Biocatalysis

M. Bekerle-Bogner, M. Gruber-Khadjawi, H. Wilsche, R. Wiedner, H. Schwab, K. Steiner*

(R)-Selective Nitroaldol Reaction Catalyzed by Metal-Dependent Bacterial Hydroxynitrile Lyases

One enzyme, two reactions: Bacterial hydroxynitrile lyases (HNLs) with a cupin fold couple nitromethane or nitroethane and aldehydes to yield (R)-β-nitro alcohols with up to 90% conversion and up to ≥ 99% enantiomeric excess.



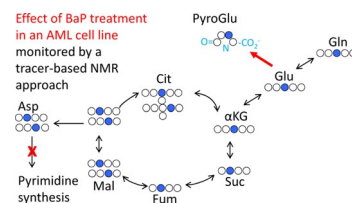


Cancer Cells

J. B. Carrigan, M. A. C. Reed, C. Ludwig, F. L. Khanim, C. M. Bunce, U. L. Günther*

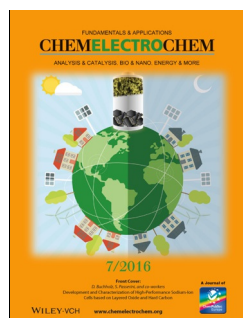
Tracer-Based Metabolic NMR-Based Flux Analysis in a Leukaemia Cell Line

Track and trace: Tracer-based metabolic analysis using NMR methods was used to identify metabolic characteristics in haematological cancer cells. Haematological cancer cells were treated with redeployed drugs (BaP=medroxyprogesterone + bezafibrate) that generate high concentrations of reactive oxygen species. NMR analysis shows how these drugs affect metabolism including the inhibition of de novo pyrimidine synthesis.



ChemPlusChem

DOI: 10.1002/cplu.201500549

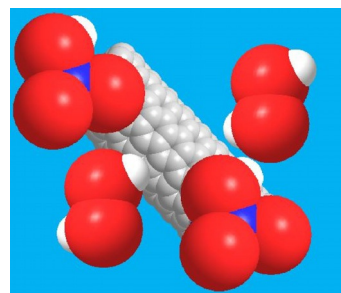


Carbon Nanotubes

R. Gusmão, Z. Sofer, M. Nováček, M. Pumera*

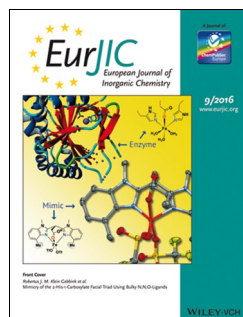
Contrasts between Mild and Harsh Oxidation of Carbon Nanotubes in Terms of Their Properties and Electrochemical Performance

Harsh reality: The modification of electrodes with carbon nanotubes (CNTs) is currently employed in numerous applications as a way to improve their performance. Here, the effects of harsh (HNO_3) and mild (H_2O_2) oxidative treatments of CNTs are highlighted. Depending on the oxidative route, their electrochemical performances are indubitably different.



ChemElectroChem

DOI: 10.1002/celc.201600082

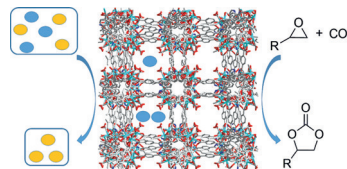


Carbon Dioxide Fixation

S. Kumar, G. Verma, W.-Y. Gao, Z. Niu, L. Wojtas, S. Ma*

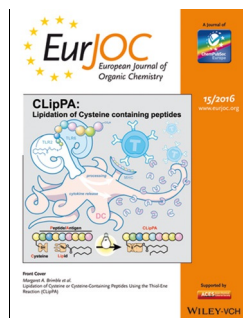
Anionic Metal–Organic Framework for Selective Dye Removal and CO_2 Fixation

A microporous Zn-based anionic metal–organic framework (MOF) is synthesized with triangular 4,4',4''-(pyridine-2,4,6-triyl)tribenzoic acid; it features open channels and proves to be a good capturing agent for cationic dyes. In addition, the Zn-MOF demonstrates excellent catalytic activity for CO_2 fixation by cycloaddition reaction with epoxides.



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201600218

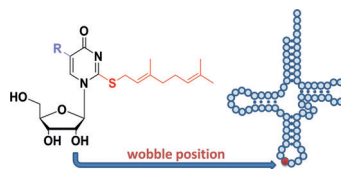


Modified Nucleosides

G. Leszczynska,* K. Sadowska, P. Bartos, B. Nawrot, E. Sochacka

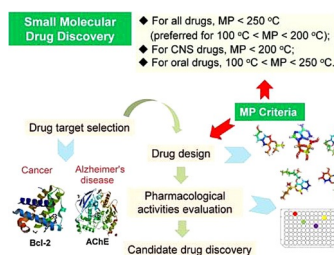
S-Geranylated 2-Thiouridines of Bacterial tRNAs: Chemical Synthesis and Physicochemical Properties

5-Substituted S-geranyl-2-thiouridines are modified nucleosides present in the first (wobble) position of bacterial tRNA anticodons. Geranylated nucleosides are obtained by S-alkylation of suitably protected 2-thiouridines. The influence of the S-geranyl moiety on the hydrophobic and conformational properties of modified nucleosides is determined and compared to that of parent 2-thiouridines.



Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201600519



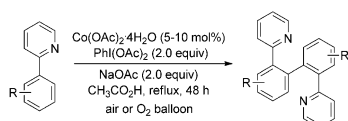
ChemistryOpen
DOI: 10.1002/open.201600015

Drug Design

F. Mao, Q. Kong, W. Ni, X. Xu, D. Ling, Z. Lu, J. Li*

Melting Point Distribution Analysis of Globally Approved and Discontinued Drugs: A Research for Improving the Chance of Success of Drug Design and Discovery

Mysteries of melting points! Herein, we report the largest melting point (MP) database (experimental value) of globally approved and discontinued drugs. We subsequently extracted six subdatabases from the “approved” database and two from the “discontinued” database and studied the MP distributions and the relationships of molecular weight versus MP, Clog *P* versus MP distributions. We revealed five noteworthy observations, hoping to provide a theoretical foundation for designing new chemical entities with good drug-like properties.



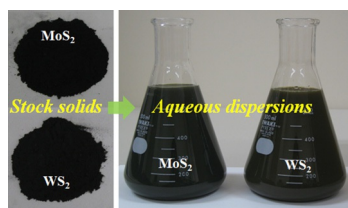
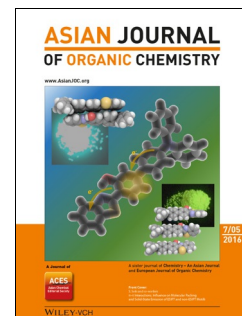
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201600241

C-H Activation

Y. Xie, D. Xu, W.-W. Sun, S.-J. Zhang, X.-P. Dong, B. Liu,* Y. Zhou,* B. Wu*

Cobalt-Catalyzed Oxidative Dimerization of 2-Phenylpyridine Derivatives

The oxidative dimerization of 2-phenylpyridine derivatives using cobalt catalysis is reported. Three types of reaction conditions were developed with different loadings of cobalt catalyst. The cross coupling of two different 2-arylpyridines using cobalt catalysis proceeded with modest yields and selectivity.



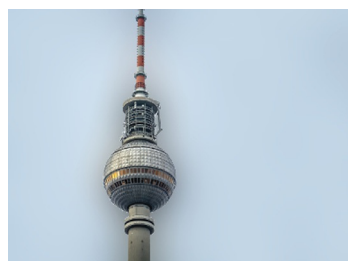
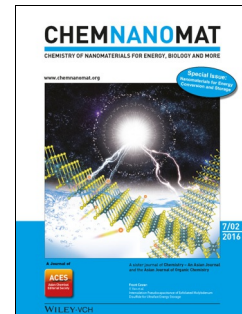
ChemNanoMat
DOI: 10.1002/cnma.201600116

Two-Dimensional Materials

G. Liu, N. Komatsu*

Readily Available “Stock Solid” of MoS₂ and WS₂ Nanosheets through Solid-Phase Exfoliation for Highly Concentrated Dispersions in Water

Readily available: A “stock solid” of MoS₂ and WS₂ nanosheets is facilely prepared through exfoliation of the bulk materials with a dry ball milling process. Since the resulting solids are very stable for long periods of time, an aqueous dispersion with the same quality and controlled concentration is available anytime simply by shaking the “stock solid” in water by hand followed by centrifuging the resulting suspension.



ChemViews magazine
DOI: 10.1002/chemv.201600041

Women in Science

V. Koester, E. Nowicka, R. Schomäcker, M. Tasbihi

Fellowship for Outstanding Female Researchers

The *International Post-Doc Initiative* (IPODI) of the Technical University of Berlin awards fellowships to outstanding female researchers. Two of them, Minoo Tasbihi from Iran and Ewa Nowicka from Poland, share their experiences in *ChemViews Magazine* and explain both their research and the challenges young scientists are facing.

