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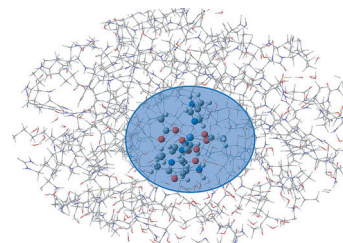


Enzymatic Processes

M. G. Quesne,* T. Borowski,* S. P. de Visser*

Quantum Mechanics/Molecular Mechanics Modeling of Enzymatic Processes: Caveats and Breakthroughs

The do's and don'ts of QM/MM: This manuscript gives a tutorial review on the challenges and caveats of running QM/MM calculations and explains the reader the key steps in the set-up processes.



Chem. Eur. J.
DOI: 10.1002/chem.201503802

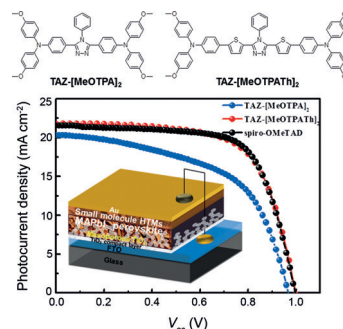


Solar Cells

H. Choi, H. Jo, S. Paek, K. Koh, H. M. Ko, J. K. Lee,* J. Ko*

Efficient Hole-Transporting Materials with Triazole Core for High-Efficiency Perovskite Solar Cells

Giving and receiving: Donor–acceptor–donor type hole-transporting materials comprising a triazole core and two electron-rich triphenylamine derivatives were successfully synthesized and characterized. Their performance in n-i-p type perovskite solar cells reached high power conversion efficiencies of up to 14.4%.



Chem. Asian J.
DOI: 10.1002/asia.201501178

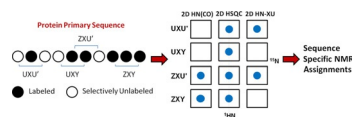


NMR Spectroscopy

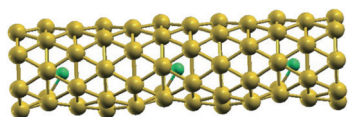
A. Dubey, R. V. Kadumuri, G. Jaipuria, R. Vadrevu,* H. S. Atreya*

Rapid NMR Assignments of Proteins by Using Optimized Combinatorial Selective Unlabeling

Removing labels: A new approach for rapid NMR assignments of proteins based on amino acid selective unlabeled is described. The method involves choosing optimal amino acids for selective unlabeled and identifying tripeptides with 2D NMR spectra in a combinatorial manner. With this approach, ~50% sequence specific assignments can be obtained directly.



ChemBioChem
DOI: 10.1002/cbic.201500513



Carbon Nanotubes

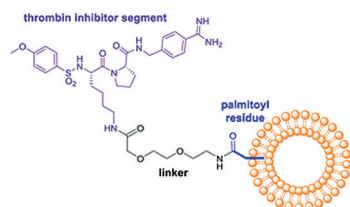
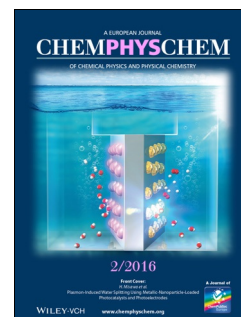
L. Mohammadzadeh, A. Goduljan, F. Juarez, P. Quaino, E. Santos, W. Schmickler*

On the Energetics of Ions in Carbon and Gold Nanotubes

The insertion of halide and alkali atoms into narrow single-walled carbon nanotubes with diameters $< 9 \text{ \AA}$ is investigated by density functional theory.

ChemPhysChem

DOI: 10.1002/cphc.201500682



Anticoagulants

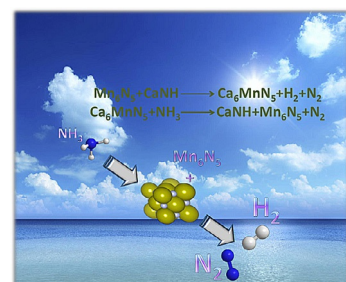
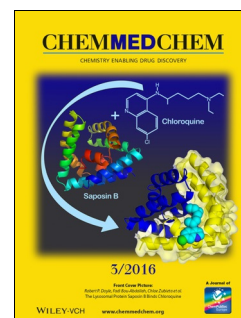
W. Endreas, J. Brüßler, D. Vornicescu, M. Keusgen, U. Bakowsky, T. Steinmetzer*

Thrombin-Inhibiting Anticoagulant Liposomes: Development and Characterization

New anticoagulant liposomes: Highly potent palmitoylated thrombin inhibitors were developed and conveniently incorporated into membranes during liposome preparation. The liposomes contain the inhibitor moiety on their surface and possess strong thrombin inhibitory potency and anticoagulant activity in plasma. This concept should be applicable to other drug molecules that suffer from rapid elimination and allow covalent modification with a suitable fatty acid residue.

ChemMedChem

DOI: 10.1002/cmdc.201500489



Hydrogen Storage

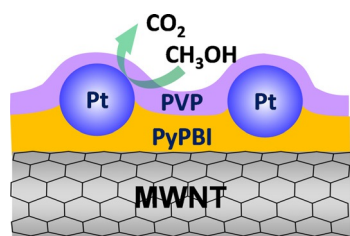
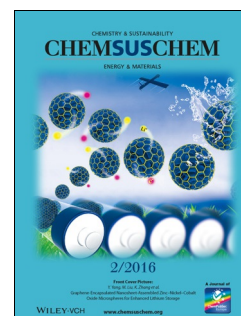
P. Yu, J. Guo, L. Liu, P. Wang, G. Wu, F. Chang, P. Chen*

Ammonia Decomposition with Manganese Nitride–Calcium Imide Composites as Efficient Catalysts

The Wrath of CaNH: Calcium imide (CaNH) has a strong synergistic effect on Mn_6N_5 in catalyzing NH_3 decomposition, leading to outstanding catalytic activity. CaNH participates in the catalysis and produces a stable $[\text{Ca}_6\text{MnN}_5]$ -like intermediate, lowering the activation energy for ammonia decomposition. A two-step catalytic cycle, accounting for the synergistic effect between CaNH and Mn_6N_5 , is proposed.

ChemSusChem

DOI: 10.1002/cssc.201501498



Electrocatalysis

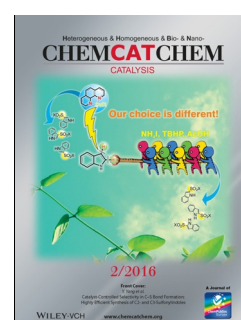
Z. Yang, N. Nakashima*

An Electrocatalyst Based on Carbon Nanotubes Coated with Poly(vinylpyrrolidone) Shows a High Tolerance to Carbon Monoxide in a Direct Methanol Fuel Cell

I'll get my coat: A poly(vinylpyrrolidone)-coated electrocatalyst assisted by polybenzimidazole showed a dramatic enhancement (10 times) of CO tolerance. PVP = poly(vinylpyrrolidone) PyPBI = poly[2,2'-(2,6-pyridine)-5,5'-bibenzimidazole]

ChemCatChem

DOI: 10.1002/cctc.201501060



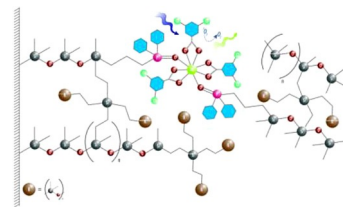


Sensors

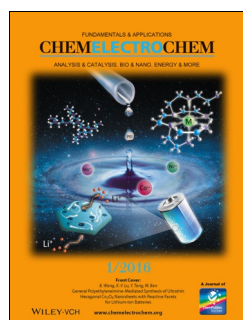
R. D. L. Gaspar, J. H. S. K. Monteiro, I. M. Raimundo, Jr., I. O. Mazali, F. A. Sigoli*

Photostable, Oxygen-Sensitive Optical Probe Based on a Homonuclear Terbium(III) Complex Covalently Bound to Functionalized Polydimethylsiloxane

Oxygen sensitive: The Tb^{III}-based sensor (see figure) showed green emission and transparency in the visible range. The optically sensitive probe was photostable under excitation at 350 nm and showed high oxygen sensitivity, I_0/I_{100} , equal to 8.9 at 1 atm. Also, its reversibility was demonstrated after several cycles ranging from 100% N₂ to 100% O₂ with response time of 8.5 s and recovery time of 49.5 s.



ChemPlusChem
DOI: 10.1002/cplu.201500296

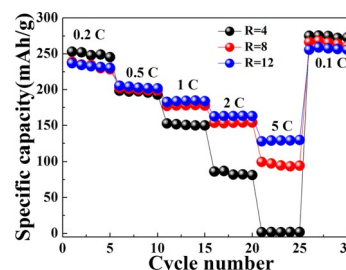


Electrode Materials

T. Zhang, J.-T. Li,* J. Liu, Y.-P. Deng, Z.-G. Wu, Z.-W. Yin, J.-H. Wu, L. Huang, S.-G. Sun*

Improving the Electrochemical Performance of Li_{1.14}Ni_{0.18}Mn_{0.62}O₂ by Modulating Structure Defects via a Molten Salt Method

Molten salt modulation: The level of Li⁺/Ni²⁺ mixing in lithium-rich cathode materials obtained by a molten salt method is affected by the amount of molten agent. The rate performance is influenced accordingly and is observed to increase at lower Li⁺/Ni²⁺ ratios.



ChemElectroChem
DOI: 10.1002/celec.201500390

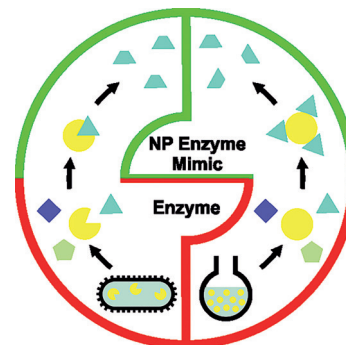


Artificial Enzymes

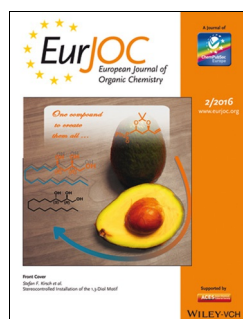
R. Ragg, M. N. Tahir, W. Tremel*

Solids Go Bio: Inorganic Nanoparticles as Enzyme Mimics

This microreview highlights the recent progress in the field of nanoparticles possessing enzyme-like activities, including peroxidase, halo-peroxidase, superoxide dismutase and sulfite oxidase mimics. Inorganic nanoparticles are more stable and cost-efficient in synthesis than their natural counterparts, while exhibiting equally high enzymatic activities.



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201501237

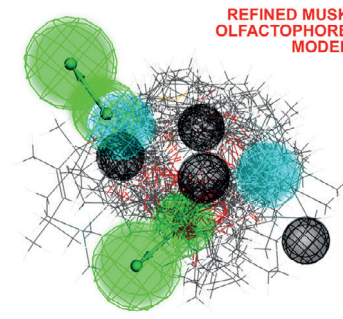


Fragrances

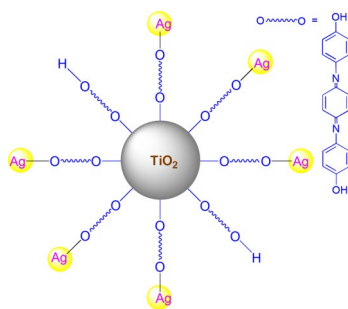
J. Liu,* Y. Zou, W. Fan, J. Mao, G. Chai, P. Li, Z. Qu, Y. Zong, J. Zhang,* P. Kraft*

Synthesis and Olfactory Properties of Silicon-Containing Analogs of Rosamusk, Romandolide, and Applelide: Insights into the Structural Parameters of Linear Alicyclic Musk

Sila-Rosamusk, sila-Romandolide, sila-Applelide, and their dehydro derivatives were synthesized from sila-analogs of Artemone and Herbac by hydride reduction and subsequent esterification. The olfactory properties of these compounds allowed a refined musk olfactophore model to be developed. The model shows that it is likely that linear and macrocyclic musks address the same odorant receptors.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201501338



ChemistryOpen

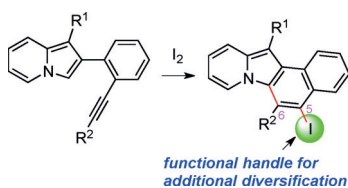
DOI: 10.1002/open.201500110

Selective Oxidation

A. Abd-Elal, F. Parrino,* R. Ciriminna, V. Loddo, L. Palmisano,* M. Pagliaro*

Alcohol-Selective Oxidation in Water under Mild Conditions via a Novel Approach to Hybrid Composite Photocatalysts

A new approach for the selective oxidation of soluble aromatic alcohols in water under mild conditions via a novel composite photocatalyst has been developed. The catalyst is synthesized by grafting an organic diol and silver nanoparticles onto the surface of titanium dioxide. The method is general and opens the route to optimization of the selective conversion for several other photocatalytic redox reactions mediated by similar advanced hybrid composites.



Asian J. Org. Chem.

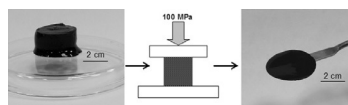
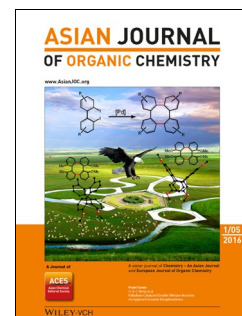
DOI: 10.1002/ajoc.201500423

Cyclization Reactions

Y. Jung, I. Kim*

Synthesis of 6-Aryl-5-iodobenzo[e]pyrido[1,2-a]indoles by 6-endo-dig Iodocyclization

Give me a ring! A range of 6-aryl-5-iodobenzo[e]pyrido[1,2-a]indoles were regioselectively synthesized by mild iodine-mediated cyclization. Further molecular diversity was achieved by reaction of the 5-iodo group in a Pd-catalyzed reaction.



ChemNanoMat

DOI: 10.1002/cnma.201500204

Supercapacitors

M. Sevilla, G. A. Ferrero, T. T. Vu, A. B. Fuentres*

A Simple Approach towards Highly Dense Solvated Graphene Films for Supercapacitors

Free-standing graphene films: Highly dense and free-standing solvated graphene films are obtained by pressing graphene hydrogels synthesized through an endotemplating approach. These films have several important properties that give rise to an excellent electrochemical performance when this type of material is used as electrodes in supercapacitors.



ChemViews magazine

DOI: 10.1002/chemv.201600001

Highlights

ChemViews

Best of 2015

2015 was *ChemistryViews'* fifth successful year online. This year's list of most popular articles was topped by education topics and stories about the chemistry of everyday life. The articles, videos, and webinars include tips on writing scientific papers and how to start a career in industry, cover the chemistry of "Breaking Bad", and explain carbonate looping technology.

