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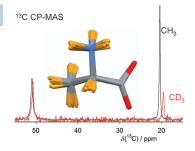


#### **Nuclear Delocalisation**

M. Dračínský,\* P. Hodgkinson\*

Effects of Quantum Nuclear Delocalisation on NMR Parameters from Path Integral Molecular Dynamics

Path finder: The influence of nuclear delocalisation on NMR chemical shifts is explored using path integral molecular dynamics and is shown to explain previously observed systematic deviations between calculated and experimental shifts (see graphic). Path integral molecular dynamics (PIMD) also enables isotope substitution effects to be predicted in excellent agreement with experiment.



Chem. Eur. J.

DOI: 10.1002/chem.201303496

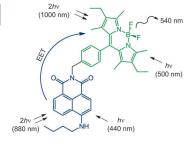


#### **Imaging Agents**

D. Collado, P. Remón, Y. Vida, F. Najera, P. Sen, U. Pischel,\* E. Perez-Inestrosa\*

Energy Transfer in Aminonaphthalimide-Boron-Dipyrromethene (BODIPY) Dyads upon One- and Two-Photon Excitation: Applications for Cellular Imaging

**Take two**: Aminonaphthalimide—BODIPY energy transfer cassettes were designed in order to take advantage for bioimaging from one-and two-photon excitation coupled with energy transfer. The bichromophoric dyads showed ultrafast and highly efficient energy transfer and were used for confocal fluorescence microscopy imaging of HeLa cells as bio-relevant models.



Chem. Asian J.

DOI: 10.1002/asia.201301334



# Glycan Microarrays

N. N. Maolanon, M. Blaise, K. K. Sørensen, M. B. Thygesen, E. Cló, J. T. Sullivan, C. W. Ronson, J. Stougaard, O. Blixt, K. J. Jensen\*

Lipochitin Oligosaccharides Immobilized through Oximes in Glycan Microarrays Bind LysM Proteins

Hold still! Complex lipochitin oligosaccharides were immobilized by oxime linkages to form a glycan microarray to evaluate binding of proteins containing LysM domains. Array functionality was evaluated by using LysM domain-containing protein autolysin p60, which targets bacterial peptidoglycan. Specific binding to Nod factors and chitin oligosaccharides was observed, with increasing affinity corresponding to increasing chitin oligomer length.

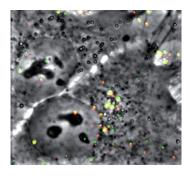


ChemBioChem

DOI: 10.1002/cbic.201300520

2024





ChemPhysChem
DOI: 10.1002/cphc.201300802

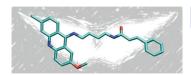
#### Fluorescent Nanodiamonds

Y. Nawa, W. Inami, S. Lin, Y. Kawata,\* S. Terakawa, C.-Y. Fang, H.-C. Chang

Multi-Color Imaging of Fluorescent Nanodiamonds in Living HeLa Cells Using Direct Electron-Beam Excitation

Live broadcast: Multi-color, high spatial resolution imaging of fluorescent nanodiamonds (FNDs) in living HeLa cells is performed with a direct electron-beam excitation-assisted fluorescence (D-EXA) microscope. Green- and red-light-emitting FNDs are employed for two-color imaging, which are observed simultaneously in the cells with high spatial resolution. This technique opens up new possibilities to reveal various cell functions by multi-color immunostaining.





#### **Antiprotozoal Agents**

A. Gomes, B. Pérez, I. Albuquerque, M. Machado, M. Prudêncio, F. Nogueira, C. Teixeira,\* P. Gomes\*

N-Cinnamoylation of Antimalarial Classics: Quinacrine Analogues with Decreased Toxicity and Dual-Stage Activity

**Reviving the classics!** Novel *N*-cinnamoylated quinacrine analogues exhibit dual-stage activity and decreased cytotoxicity. Given the emergence of *P. falciparum* resistant to long-established acridine-based drugs such as quinacrine, these findings could lead the way for the "rise of a fallen angel" in antimalarial chemotherapy.



ChemMedChem

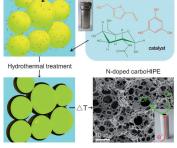
DOI: 10.1002/cmdc.201300459



Biosourced Nitrogen-Doped Microcellular Carbon Monoliths

Mega monoliths: An original approach to synthesize nitrogen-doped microcellular carbon monoliths based on the hydrothermal carbonization of N-containing biomass derivatives is reported. Monosaccharides could be directly used as precursors, enhancing the sustainability of the approach. These biosourced foams show promising performances as intrinsic electrocatalysts in the oxygen reduction reaction.





ChemSusChem
DOI: 10.1002/cssc.201301165

# 80 isomerization selectivity Pdi //SAIF<sub>3</sub> 20 conversion 80 isomerization selectivity PU //SAIF<sub>3</sub> Conversion

ChemCatChem
DOI: 10.1002/cctc.201300840

#### Hydroisomerization

Carbon Catalysis

O. Machynskyy, E. Kemnitz,\* Z. Karpiński\*

Aluminum Fluoride-Supported Platinum and Palladium as Highly Efficient Catalysts of *n*-Pentane Hydroisomerization

A week-long performance: High surface area (HS) aluminum fluoride-supported palladium and platinum catalysts are used in the isomerization of n-pentane. The activity, stability, and selectivity of Pt/HS-AlF3 and Pd/HS-AlF3 catalysts is maintained at temperatures of up to 350 °C over reaction times of up to a week. Both Lewis and Brønsted acidity is detected in the activated catalysts, evidencing bifunctional isomerization.







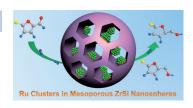


#### **Batteries**

H. Li, L. Shen, J. Wang, B. Ding, P. Nie, G. Xu, X. Wang, X. Zhang\*

Design of a Nitrogen-Doped, Carbon-Coated  $\rm Li_4Ti_5O_{12}$  Nanocomposite with a Core–Shell Structure and Its Application for High-Rate Lithium-Ion Batteries

**Made to fit**: A nitrogen-doped, carbon-coated  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  nanocomposite with a core–shell structure has been synthesized using the ionic liquid 1-ethyl-3-methylimdazolium tricyanomethanide as the carbon source. The well-defined nanocomposite displays better cycling and rate performances than those of  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  nanoparticles, and has a superior lithium-storage capability even at high rates (see picture).



ChemPlusChem

DOI: 10.1002/cplu.201300316

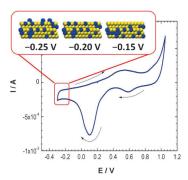


## Surface Science

M. Okube, V. Petrykin, J. E. Mueller, D. Fantauzzi, P. Krtil,\* T. Jacob\*

Topologically Sensitive Surface Segregations of Au–Pd Alloys in Electrocatalytic Hydrogen Evolution

A dynamic catalyst: DFT-based calculations along with in situ X-ray absorption spectroscopy data show that AuPd alloys form unique potential-controlled surface structures during hydrogen adsorption/evolution. Surface segregations take place, with a preference for a gold surface if the surface is free of chemisorbed species, while hydrogen adsorption triggers palladium segregation into the surface.



ChemElectroChem

DOI: 10.1002/celc.201300112

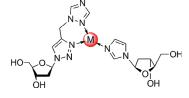


#### Metal-Mediated Base Pairs

T. Richters, J. Müller\*

A Metal-Mediated Base Pair with a [2+1] Coordination Environment

A metal-mediated base pair purely based on azole-derived ligands has been devised. It enables a [2+1] coordination environment. A DNA duplex comprising one such base pair is significantly stabilized in the presence of silver(I).



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201301491

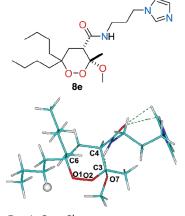


# 1,2-Dioxanes

M. Lombardo,\* D. P. Sonawane, A. Quintavalla, C. Trombini, D. D. Dhavale, D. Taramelli, Y. Corbett, F. Rondinelli, C. Fattorusso,\* M. Persico, O. Taglialatela-Scafati

Optimized Synthesis and Antimalarial Activity of 1,2-Dioxane-4-carboxamides

An optimized two-step protocol for the synthesis of 3-methoxy-4-methoxycarbonyl-1,2-dioxanes is reported. This approach is exploited for the synthesis of a new family of 4-carboxamide derivatives with interesting antimalarial activities.

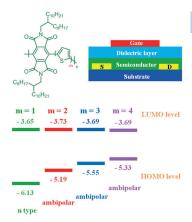


Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201301394

# on our Sister Journals





Asian J. Org. Chem.

DOI: 10.1002/ajoc.201300228

## **Conjugated Polymers**

Switchable-Hydrophilicity Solvents

X. Zhou, Y. Cao, X.-Y. Wang, Z.-H. Guo, J.-Y. Wang,\* J. Pei\*

Tuning the Charge-Transport Property of Pyromellitic Diimide-Based Conjugated Polymers towards Efficient Field-Effect Transistors

More thiophene please! A series of donor-acceptor conjugated polymers were synthesized that include pyromellitic diimide (PMDI) as the acceptor and thiophene as the donor unit. With different thiophene/PMDI ratios in the polymer chains, the photophysical and electrochemical properties varied, and the field-effect transistors changed from n-type to ambipolar. Furthermore, with more thiophene, the hole mobilities of these polymers increased.





ChemViews magazine
DOI: 10.1002/chemv.201300139

# David Bradley

Finding a New Solution to Chemical Problems

Volatile organic solvents (VOCs) are widely used by chemists but are flammable and can be toxic. David Bradley discusses a potential greener, less toxic alternative. Switchable-hydrophilicity solvents (SHSs), developed by Canadian chemists, are miscible with water in one form but not in another and can be separated without distillation. New SHSs are potentially safer for the environment than VOCs.

