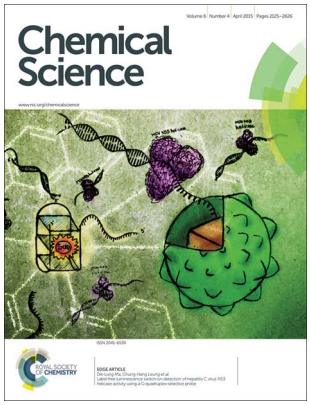
Chemical Science

www.rsc.org/chemicalscience

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

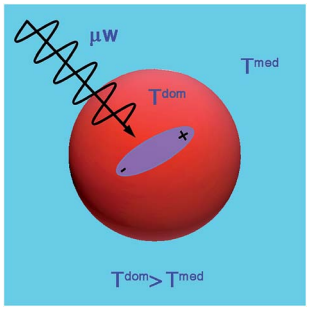
ISSN 2041-6539 CODEN CSHCBM 6(4) 2125–2626 (2015)



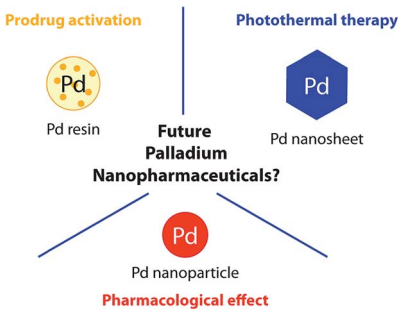
Cover
See Dik-Lung Ma, Chung-Hang Leung *et al.*, pp. 2166–2171.
Image reproduced by permission of Dik-Lung Ma from *Chem. Sci.*, 2015, **6**, 2166.

Inside cover
See Basile Commarieu and Jerome P. Claverie, pp. 2172–2181.
Image reproduced by permission of Jerome P. Claverie from *Chem. Sci.*, 2015, **6**, 2172.

PERSPECTIVE



MINIREVIEWS



Editorial staff

Interim executive editor
May Copsey

Deputy editor
Jeanne Andres

Editorial production manager
Philippa Ross

Development editors
Alessia Millemaggi
Cesar Palmero

Publishing editors
Matthew Bown, Sage Bowser, Hugh Cowley, Ruth Dilleen, Cally Haynes, Alan Holder, Samantha Ivell, James Moore, Liisa Niitsoo, Victoria Richards, Susan Weatherby, Rachel Wood

Publishing assistants
Natalie Ford, Bethany Johnson, Rebecca Wojturska

Publisher
Jamie Humphrey

For queries about submitted articles please contact Philippa Ross, Editorial production manager, in the first instance. E-mail **chemicalscience@rsc.org**

For pre-submission queries please contact May Copsey, Interim executive editor. E-mail **chemicalscience-rsc@rsc.org**

Chemical Science (electronic: ISSN 2041-6539) is published monthly by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read. Please email **orders@rsc.org** to register your interest or contact RSC Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail **orders@rsc.org**

Advertisement sales: Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail **advertising@rsc.org**

For marketing opportunities relating to this journal, contact **marketing@rsc.org**

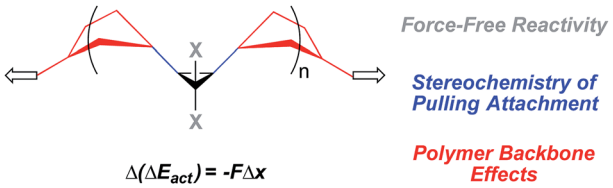
Chemical Science

www.rsc.org/chemicalscience

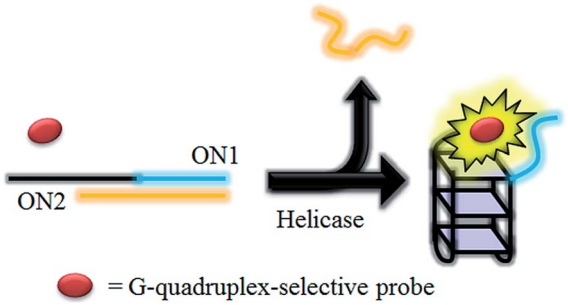
Information for authors

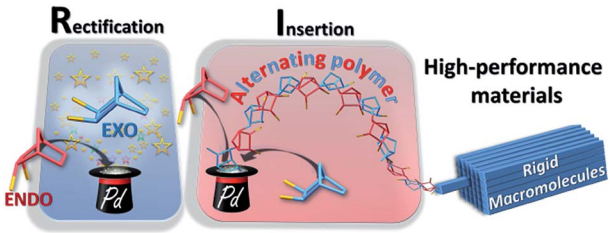
Full details on how to submit material for publication in Chemical Science are given in the Instructions for Authors (available from **http://www.rsc.org/authors**). Submissions should be made via the journal's homepage: **http://www.rsc.org/chemicalscience**.

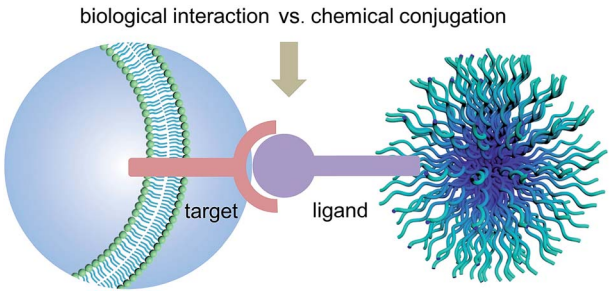
MINIREVIEWS



EDGE ARTICLES

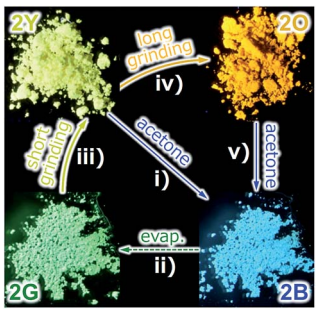






EDGE ARTICLES

2187

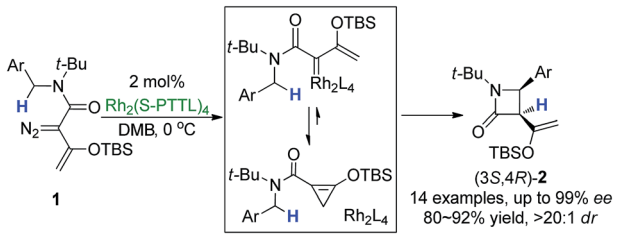


Interconvertible multiple photoluminescence color of a gold(I) isocyanide complex in the solid state: solvent-induced blue-shifted and mechano-responsive red-shifted photoluminescence

Tomohiro Seki, Taichi Ozaki, Takuma Okura, Kiyotaka Asakura, Aya Sakon, Hidehiro Uekusa* and Hajime Ito*

We report the first example of a mechanochromic compound that can switch between four individual types of photoluminescence in the solid state.

2196

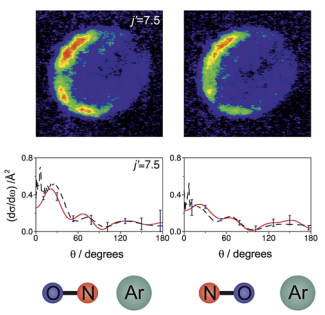


Enantioselective *cis*-β-lactam synthesis by intramolecular C–H functionalization from enoldiazoacetamides and derivative donor–acceptor cyclopropenes

Xinfang Xu,* Yongming Deng, David N. Yim, Peter Y. Zavalij and Michael P. Doyle*

β-Lactam derivatives are produced through donor–acceptor cyclopropene intermediates in high yield with exclusive *cis*-diastereoselectivity, and high enantiocontrol.

2202

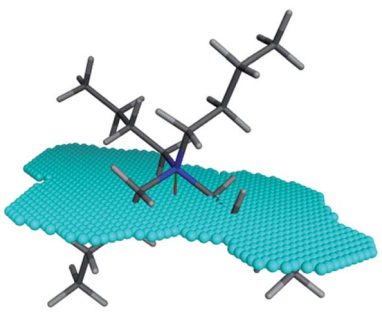


Steric effects and quantum interference in the inelastic scattering of NO(X) + Ar

B. Nichols, H. Chadwick, S. D. S. Gordon, C. J. Eyles, B. Hornung, M. Brouard,* M. H. Alexander, F. J. Aoiz, A. Gijsbertsen and S. Stolte

New measurements of the differential steric effect for NO + Ar inelastic scattering highlight the importance of quantum interference.

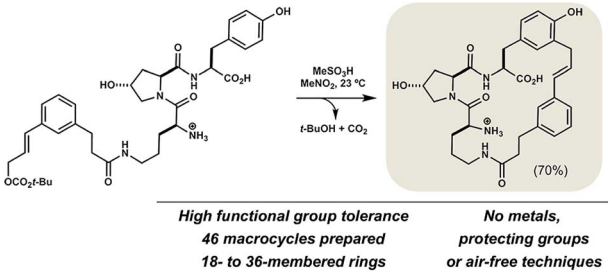
2211

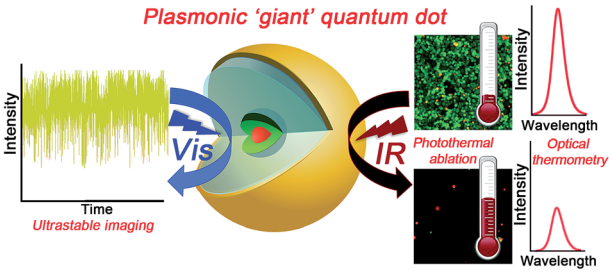


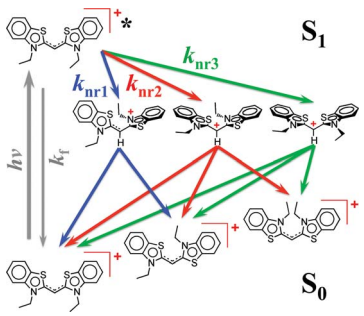
Redefining *q*: quaternary ammonium cross sectional area (XSA) as a general descriptor for transport-limiting PTC rate approximations

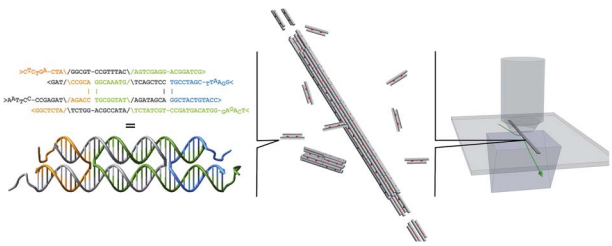
S. E. Denmark* and J. J. Henle

Several descriptors were studied in transport-rate limiting PTC, with amphiphilic cross-sectional area (XSA) identified as a single-descriptor model of rate.



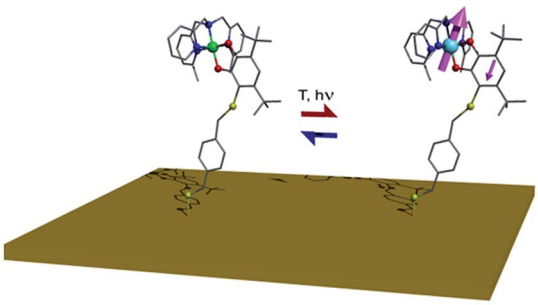






EDGE ARTICLES

2268

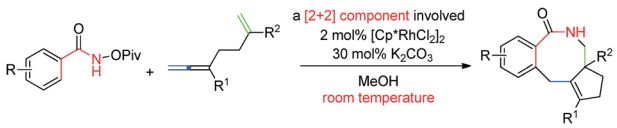


Thermal and optical control of electronic states in a single layer of switchable paramagnetic molecules

Giordano Poneti,* Lorenzo Poggini, Matteo Mannini,* Brunetto Cortigiani, Lorenzo Sorace, Edwige Otero, Philippe Sainctavit, Agnese Magnani, Roberta Sessoli and Andrea Dei

Thermally and optically induced Valence Tautomeric interconversion has been observed for a monolayer of a cobalt–dioxolene complex on gold.

2275

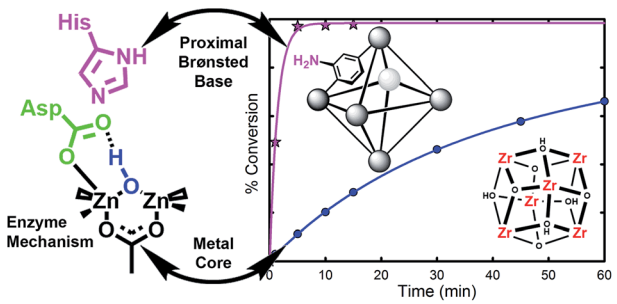


Rhodium-catalyzed C–H functionalization-based approach to eight-membered lactams

Shangze Wu, Rong Zeng, Chunling Fu, Yihua Yu, Xue Zhang* and Shengming Ma*

Fused tricyclic skeleton in one shot: a Rh^{III} catalyzed formal [4 + 2 + 2] cyclization of *N*-pivaloyloxybenzamides **1** with 1,6-allene-enes **2** adding two cycles to the benzene ring compatible with ambient air and moisture with a tolerance of many synthetic useful functional groups at room temperature have been developed.

2286

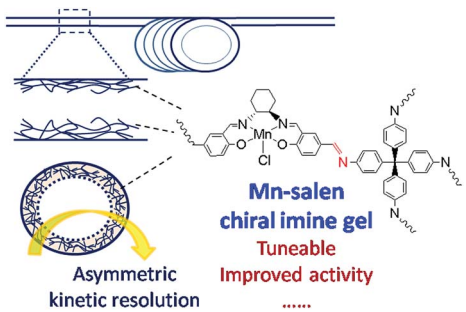


Exploiting parameter space in MOFs: a 20-fold enhancement of phosphate-ester hydrolysis with UiO-66-NH_2

Michael J. Katz, Su-Young Moon, Joseph E. Mondloch, M. Hassan Beyzavi, Casey J. Stephenson, Joseph T. Hupp* and Omar K. Farha*

Using the enzymatic mechanism of phosphoesterase as a template, we were able to modify a metal–organic framework such that the hydrolysis rates were 50 times faster than previously demonstrated with UiO-66.

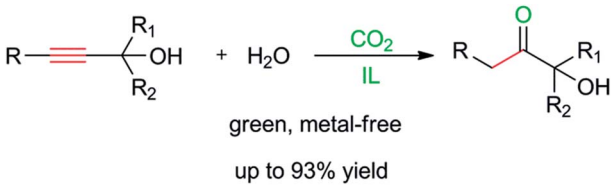
2292

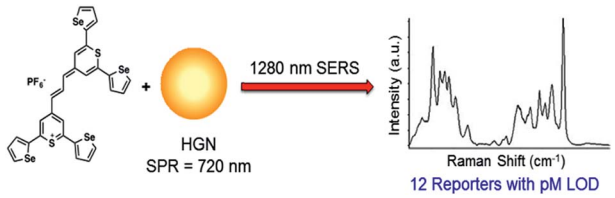


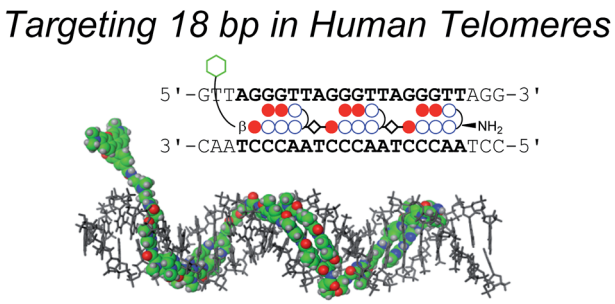
A catalytic chiral gel microfluidic reactor assembled *via* dynamic covalent chemistry

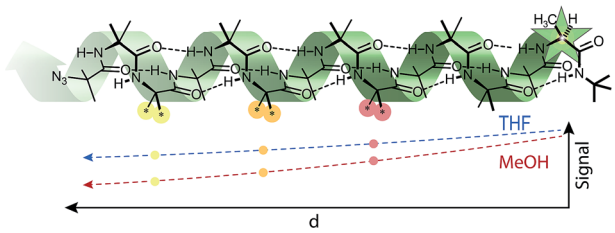
Haoliang Liu, Juan Feng, Jianyong Zhang,* Philip W. Miller,* Liuping Chen and Cheng-Yong Su*

A novel dynamic covalent gel strategy is reported to immobilize an asymmetric catalyst within the channels of a microfluidic flow reactor.

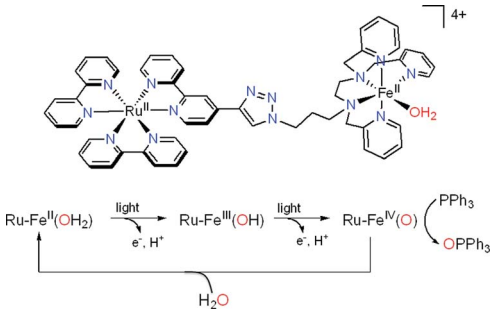








2323

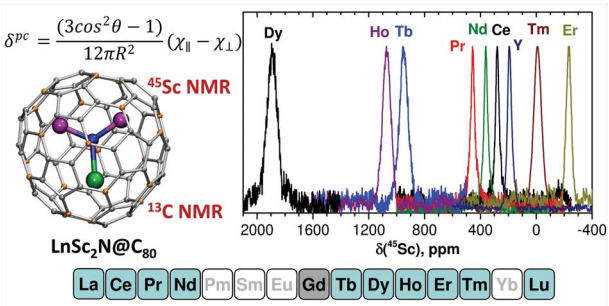


Successive light-induced two electron transfers in a Ru–Fe supramolecular assembly: from Ru–Fe(II)–OH_2 to Ru–Fe(IV)–oxo

C. Herrero, A. Quaranta, M. Sircoglou, K. Sénéchal-David, A. Baron, I. Marín, C. Buron, J.-P. Baltaze, W. Leibl,* A. Aukauloo* and F. Banse*

A Ru^{II}–Fe^{II} chromophore–catalyst assembly performs the visible-light activation of a metal-bound water molecule to form a metal oxo species responsible for the oxidation of a substrate.

2328

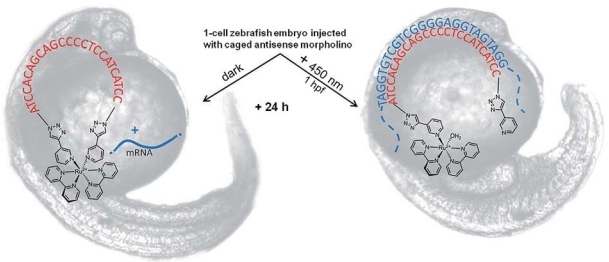


Magnetic anisotropy of endohedral lanthanide ions: paramagnetic NMR study of $MSc_2N@C_{80}$-I_h with M running through the whole 4f row

Y. Zhang, D. Krylov, M. Rosenkranz, S. Schiemenz and A. A. Popov*

Paramagnetic and variable temperature ^{13}C and ^{45}Sc nuclear magnetic resonance studies are performed for nitride clusterfullerenes $MSc_2N@C_{80}$ with icosahedral $I_h(7)$ carbon cage, where M runs through all lanthanides forming nitride clusters.

2342

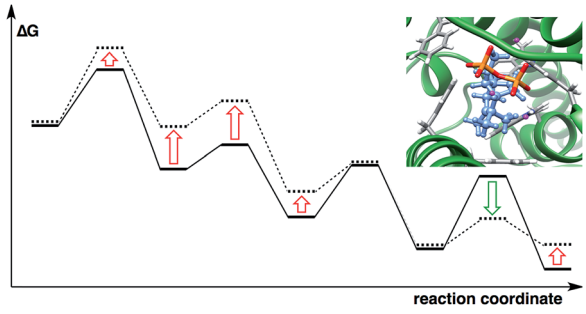


Ruthenium-caged antisense morpholinos for regulating gene expression in zebrafish embryos

Julianne C. Griepenburg, Teresa L. Rapp, Patrick J. Carroll, James Eberwine and Ivan J. Dmochowski*

Ruthenium photolinkers provide a versatile method of using visible light to control structure and function of biopolymers.

2347

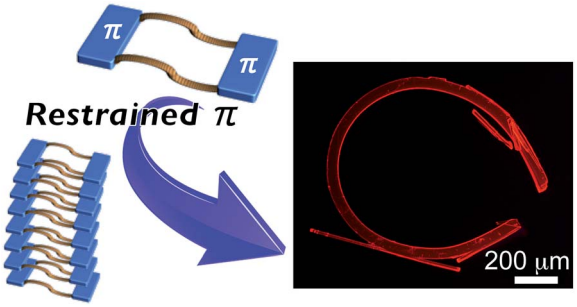


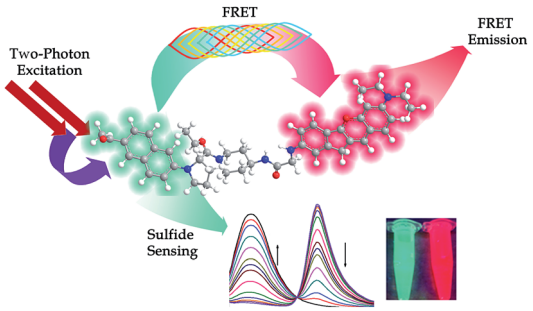
Modulation of inherent dynamical tendencies of the bisabolyl cation *via* preorganization in *epi*-isozizaene synthase

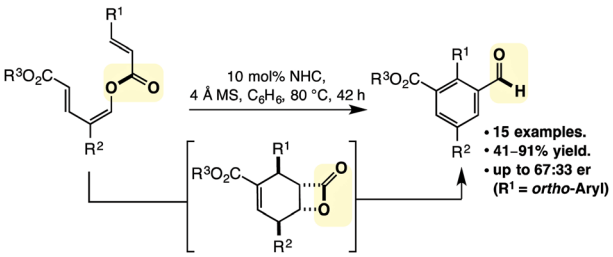
Ryan P. Pemberton, Krystina C. Ho and Dean J. Tantillo*

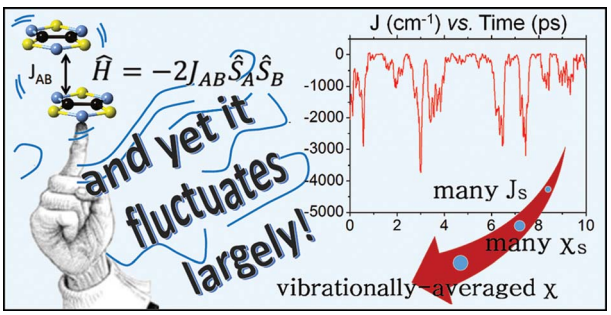
The relative importance of various factors controlling the product distribution for a terpene synthase are elucidated through a combination of quantum chemical, dynamics and automated docking calculations.

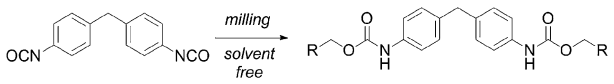
EDGE ARTICLES







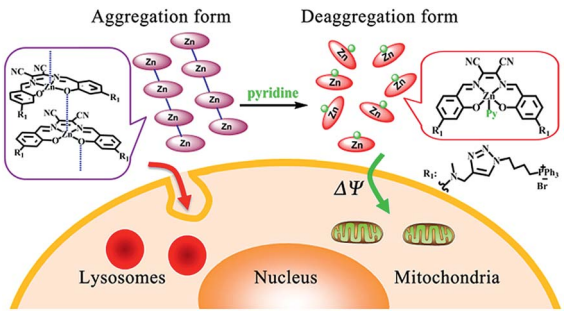




Development of solvent-free synthesis of hydrogen-bonded supramolecular polyurethanes

Kelly. A. Houton, George M. Burslem and Andrew. J. Wilson*

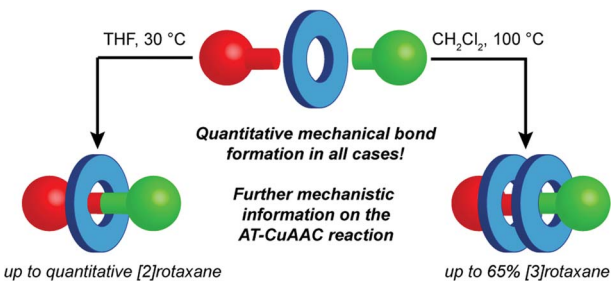
A solvent free ball-milling method for the synthesis of small molecule and oligomeric carbamates is described that is applicable to supramolecular polymer synthesis.



Unravelling the correlation between metal induced aggregation and cellular uptake/subcellular localization of Znsalen: an overlooked rule for design of luminescent metal probes

Juan Tang, Yuan-Bo Cai, Jing Jing and Jun-Long Zhang*

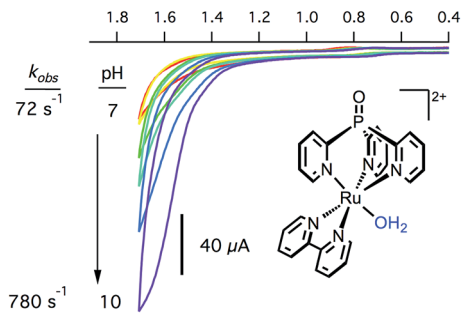
We demonstrate the importance of speciation of luminescent metal complexes in water on biological behaviours such as cellular uptake and subcellular localization.



Competitive formation of homocircuit [3]rotaxanes in synthetically useful yields in the bipyridine-mediated active template CuAAC reaction

Edward A. Neal and Stephen M. Goldup*

We demonstrate that, depending on reaction conditions, [2]rotaxanes are produced in essentially quantitative yield in the AT-CuAAC reaction regardless of macrocycle size, and hard to access doubly threaded [3]rotaxanes can be synthesised in up to 50% isolated yield in a four component coupling step.

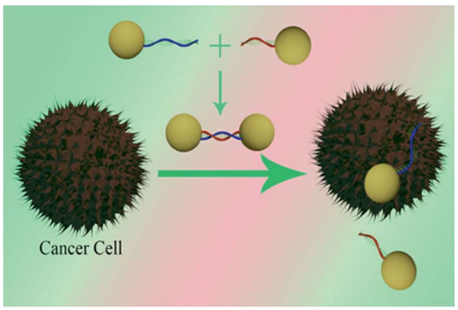


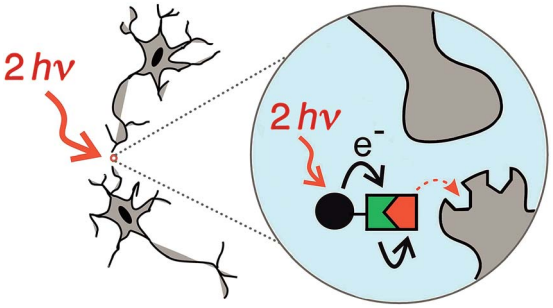
Rapid water oxidation electrocatalysis by a ruthenium complex of the tripodal ligand tris(2-pyridyl)phosphine oxide

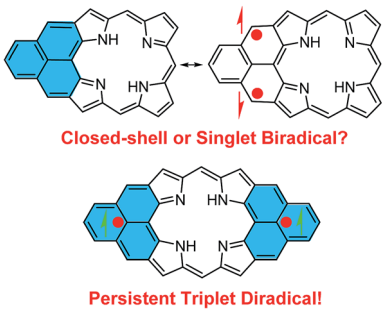
Andrew G. Walden and Alexander J. M. Miller*

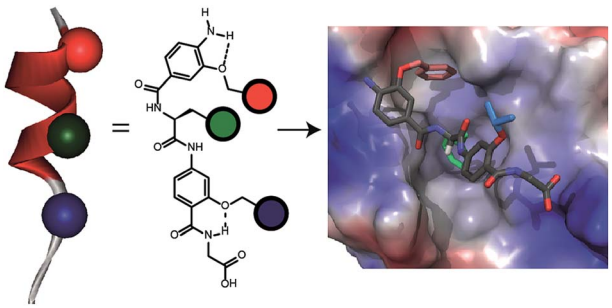
A ruthenium complex of the tripodal ligand tris(2-pyridyl)-phosphine oxide exhibits rapid water oxidation electrocatalysis over a wide pH range.

EDGE ARTICLES



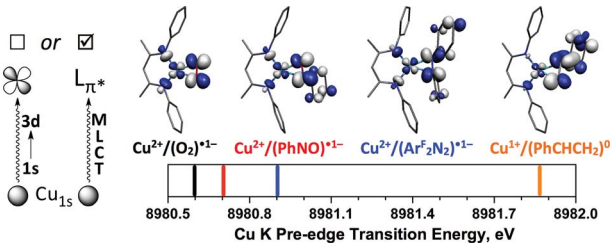


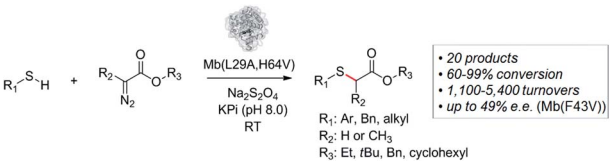


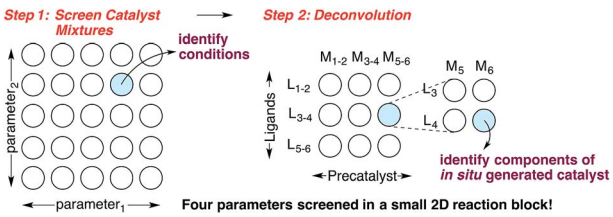


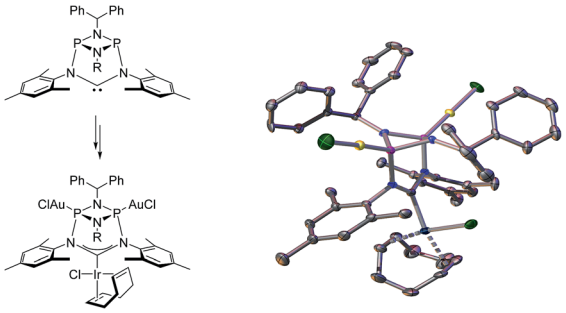
EDGE ARTICLES

EDGE ARTICLES





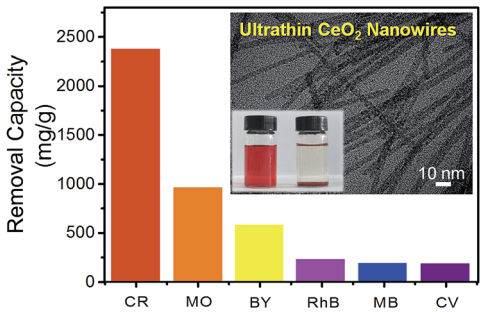




Extending *N*-heterocyclic carbene ligands into the third dimension: a new type of hybrid phosphazane/NHC system

Torsten Roth, Vladislav Vasilenko, Callum G. M. Benson, Hubert Wadepohl, Dominic S. Wright* and Lutz H. Gade*

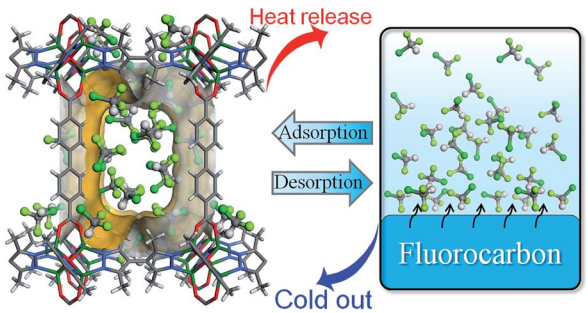
A new type of hybrid phosph(III)azane/NHC system is described in which a phosphazane P_2N_2 ring provides unique opportunities for modifying the electronic and steric character of these carbenes.



Template- and surfactant-free synthesis of ultrathin CeO_2 nanowires in a mixed solvent and their superior adsorption capability for water treatment

Xiao-Fang Yu, Jian-Wei Liu, Huai-Ping Cong, Lei Xue, Muhammad Nadeem Arshad, Hassan A. Albar, Tariq R. Sobahi, Qiang Gao and Shu-Hong Yu*

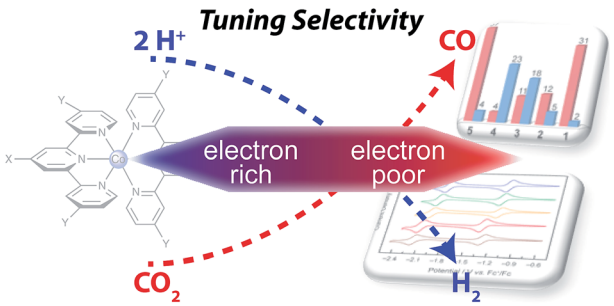
Ultrathin CeO_2 nanowires can be prepared by a one-step refluxing approach in a mixed solvent without any templates or surfactants, and exhibit excellent adsorption capabilities in water treatment.



Tuning fluorocarbon adsorption in new isoreticular porous coordination frameworks for heat transformation applications

Rui-Biao Lin, Tai-Yang Li, Hao-Long Zhou, Chun-Ting He, Jie-Peng Zhang* and Xiao-Ming Chen

We report adsorption behaviors of a typical fluorocarbon R22 ($CHClF_2$) in a new series of isoreticular porous coordination frameworks [$Zn_4O(bpz)_2(ldc)$].

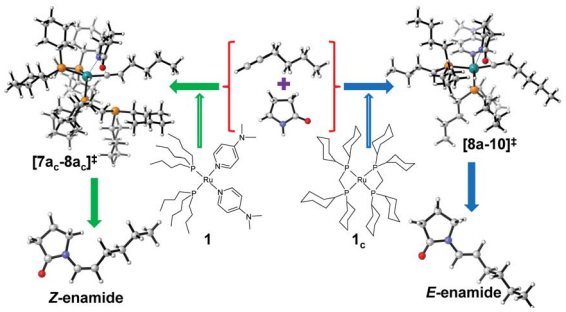


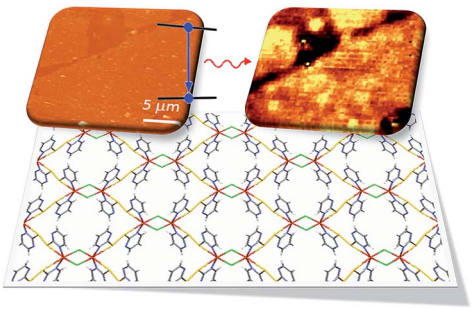
Turning it off! Disfavouring hydrogen evolution to enhance selectivity for CO production during homogeneous CO_2 reduction by cobalt–terpyridine complexes

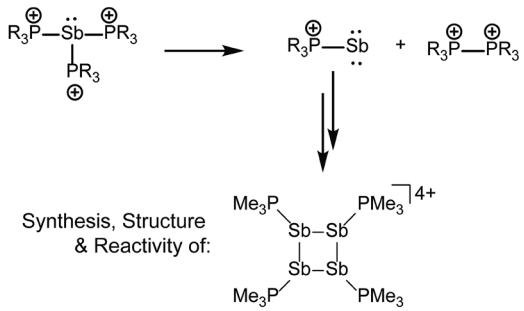
Noémie Elgrishi, Matthew B. Chambers and Marc Fontecave*

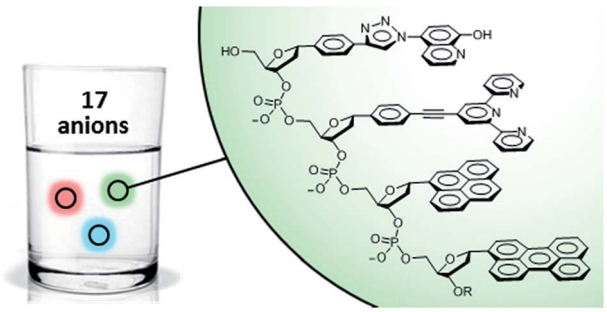
Understanding the activity and selectivity of molecular catalysts for CO_2 reduction to fuels is an important scientific endeavour in addressing the growing global energy demand.

EDGE ARTICLES









EDGE ARTICLES

EDGE ARTICLES