# NJC

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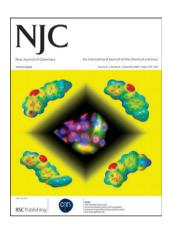
#### IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 33(9) 1793-1980 (2009)



#### Cover

See Cédric-Olivier Turrin et al., pp. 1809-1824. The painting on this Attic red-figure skyphos (ancient Greek two-handled deep wine-cup) represents a winged female figure, probably Iris, holding a caduceus (Greek vase painter, between 470 and 450 BC at Athens). The vase is in the cabinet des médailles de la Bibliothèque nationale de France, Paris, France. Photo by Bibi Saint-Pol (http://commons.wikimedia.org/ wiki/File:Winged\_goddess\_Cdm\_ Paris\_841.jpg) with permission from Olivier Rolland, Cédric-Olivier Turrin, Anne-Marie Caminade and Jean-Pierre Majoral, New J. Chem., 2009, 33, 1809.



#### Inside cover

See Colin Llewellyn Raston et al., pp. 1869-1873. Chalcones down-regulate thrombin-mediated interleukin-6 and interleukin-8 release from A549 lung epithelial cells in a dose-dependent manner. Computational analyses show that planarity and electron deficient and carbonyl carbons could be critical to their mechanism of action. The cover artwork shows Molecular Electrostatic Potential (MFP) maps of the chalcones and confocal images of the lung epithelial cells. Image reproduced by permission of Nicole Maria Smith, Pengkai Soh, Nithiananthan Asokananthan, Marck Norret, Geoffrey A. Stewart

and Colin Llewellyn Raston from

New J. Chem., 2009, 33, 1869.

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September 2009/Volume 6/Issue 9

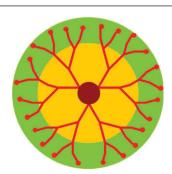
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#### **PERSPECTIVE**

1809

#### Dendrimers and nanomedicine: multivalency in action

Olivier Rolland, Cédric-Olivier Turrin,\*
Anne-Marie Caminade and Jean-Pierre Majoral
This Perspective explores the contribution of dendrimers
to the field of nanomedicine.



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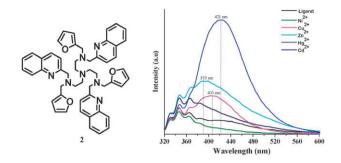


1825

A new chemosensor that signals Hg(II), Cu(II) and Zn(II) at different emission wavelengths: selectivity toward Hg(II) in acetonitrile

B. Nisar Ahamed, I. Ravikumar and Pradyut Ghosh\*

A new tripodal fluoroionophore senses  $Hg^{2+}$ ,  $Cu^{2+}$  and  $Zn^{2+}$  in acetonitrile by displaying enhanced fluorescence at distinct wavelengths and it also shows selectivity toward  $Hg^{2+}$ .



1829

### Red shining silica: macroscopic pigments and nanoparticles by silylation

Heinz Langhals,\* Andreas J. Esterbauer and Simon Kinzel Red shining perylene fluorescent dyes were obtained by their lateral extension with imidazole attached with methoxysilanes and applied for the grafting of silica nanoparticles.



1833

### Theoretical proposal for an organometallic route to cis-peptides

Robin Chaudret, Georges Trinquier, Romuald Poteau\* and Laurent Maron

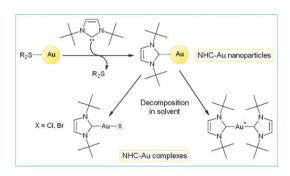
We show by means of quantum chemistry calculations that organolanthanide catalysis can be a way to obtain *cis*-amide bonds, thus providing clues for the synthesis of new peptidic materials.



#### N-Heterocyclic carbene coated metal nanoparticles

Eleanor C. Hurst, Karen Wilson, Ian J. S. Fairlamb\* and Victor Chechik\*

*N*-Heterocyclic carbene coated Au and Pd nanoparticles have been prepared by a ligand exchange reaction; although carbenes quantitatively displaced the thioether and phosphine ligands from the nanoparticle surface, the resultant nanoparticles spontaneously leached metal complexes and aggregated in solution.



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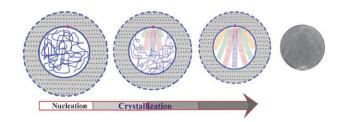


#### 1841

#### Integrated polymer spherulites growing from one homogeneous nucleation site in supercritical fluid

Changming Wang, Ying Zhao, Jinliang Song, Buxing Han and Dujin Wang\*

Integrated micro-sized spherulites of ultrahigh molecular weight polyethylene, with one clear homogeneous nucleation site and sheaf-like lamellae, have been successfully prepared from supercritical fluid of ethanol, supplying a propagating stage from sheaf-like dendrite to final spherical crystal.



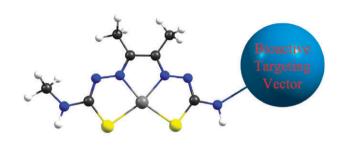
#### **PAPERS**

#### 1845

# Functionalised copper-64 complexes as precursors of potential PET imaging agents for neurodegenerative disorders

Jason P. Holland,\* Michael W. Jones, Paul D. Bonnitcha, Jason S. Lewis and Jonathan R. Dilworth

Metal bis(thiosemicarbazonato) complexes functionalised with dopamine- and tropinone-like groups have been synthesised as potential precursors towards the development of copper-based radiopharmaceuticals for *in vivo* imaging of neurodegenerative disorders.



#### 1853

# Bimetallic Cu<sup>2+</sup> complexes of bis-terpyridine ligands as catalysts of the cleavage of mRNA 5'-cap models. The effect of linker length and base moiety

Leena Maanpää, Vincent Luzet, Glemence Guillaume, Sharmin Taherpour, Esa Mäki and Satu Mikkola\*

Up to  $5 \times 10^5$  fold rate-enhancement of the cleavage of dinucleoside triphosphates is achieved with bimetallic Cu<sup>2+</sup> complexes of bis-TerPy ligands where n > 3.

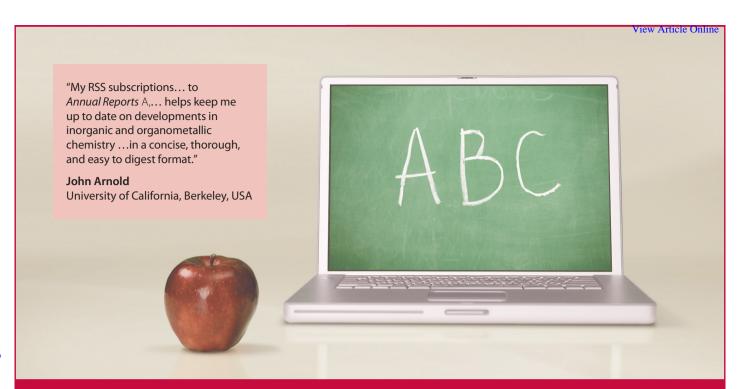
#### 1859

### Furan containing ammonium salts from furfural: synthesis and properties evaluation

Paola Galletti,\* Adele Montecavalli, Fabio Moretti, Andrea Pasteris, Chiara Samorí\* and Emilio Tagliavini

The synthesis of furan-containing quaternary ammonium salts starting from furfural has been developed combining two "green" features: the use of renewable resources with mild operation conditions.

 $R, R^1, R^2 = methyl, butyl, hexyl, octyl, dodecyl X = I, NTf<sub>2</sub>, BF<sub>4</sub>$ 



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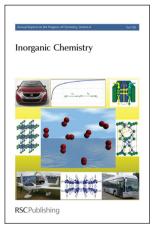
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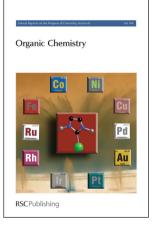
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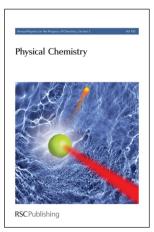
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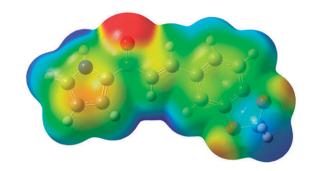


#### 1869

#### Immunomodulatory effects of functionalised chalcones on pro-inflammatory cytokine release from lung epithelial cells

Nicole Maria Smith, Pengkai Soh, Nithiananthan Asokananthan, Marck Norret, Geoffrey A. Stewart\* and Colin Llewellyn Raston\*

Chalcones down-regulate thrombin-mediated interleukin-6 and interleukin-8 release from A549 lung epithelial cells in a dose-dependent manner. Computational analyses show that planarity and electron deficient \( \beta \) and carbonyl carbons could be critical to their mechanism of action.

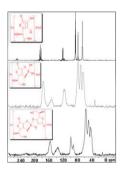


#### 1874

#### Complexation of boric acid with vitamin C

Dursun Ali Köse and Birgül Zümreoglu-Karan\*

Mono-chelate (1:1) and bis-chelate (1:2) anionic complexes of boric acid with vitamin C (L-ascorbic acid) were isolated from aqueous solutions in salt form and characterized by FTIR, <sup>13</sup>C and <sup>11</sup>B MAS NMR.

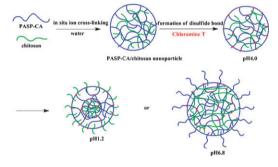


#### 1882

#### Disulfide cross-linked biodegradable polyelectrolyte nanoparticles for the oral delivery of protein drugs

Shujun Shu, Xin Wang, Xinge Zhang,\* Xuejiao Zhang, Zhen Wang and Chaoxing Li\*

Disulfide bond cross-linked nanoparticles can stack tightly at pH 1.2 and decrease the loss of protein drugs, and can swell and release the drugs slowly in an environment at pH 6.8.



#### 1888

#### A selective fluorescent sensor for imaging Cu<sup>2+</sup> in living cells

Lijuan Jiao,\* Jilong Li, Shengzhou Zhang, Chao Wei, Erhong Hao and M. Graça H. Vicente

A new membrane-permeable highly Cu<sup>2+</sup>-sensitive and selective fluorescence sensor (BODIPY 1) has been synthesized from novel 3,5-diiodo-BODIPY 4 and is suitable for intracellular imaging of Cu<sup>2+</sup> in living biological samples.



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#### **PAPERS**



The crystal structure and evidence of the phase transition in D-amphetamine sulfate, as studied by X-ray crystallography, DSC and NMR spectroscopy

Katarzyna Pogorzelec-Glaser, Joanna Kaszyńska, Adam Rachocki, Jadwiga Tritt-Goc, Narcyz Piślewski and Adam Pietraszko\*

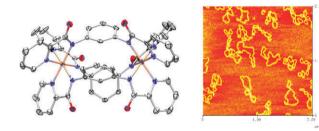
D-Amphetamine sulfate undergoes a phase transition at about 325 K, as shown by X-ray crystallography, DSC and NMR spectroscopy measurements.

#### 1901

Double and triple stranded mesocates containing the bis(bidentate) bridging ligand 1,3-bis(pyridine-2-carboxamide)benzene. Structure, properties and DNA interaction

M<sup>a</sup>Angeles Palacios, Antonio Rodríguez-Diéguez, Angelo Sironi, Juan Manuel Herrera, Antonio J. Mota, Virtudes Moreno, Joan Cano and Enrique Colacio\*

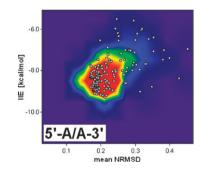
Double stranded Cu<sup>II</sup><sub>2</sub> and triple stranded Ni<sup>II</sup><sub>2</sub> meso-helicates exhibit weak ferromagnetic coupling while triple stranded Ni<sup>II</sup><sub>2</sub> and Zn<sup>II</sup><sub>2</sub> complexes interact with pBR322 DNA producing supercoiled forms, kinks and cross linking.



Intra-strand stacking interactions in B-DNA crystals characterized by post-SCF quantum chemistry computations

Piotr Cysewski\*

Structural heterogeneities of local B-DNA conformations impose only minor diversities of intra-strand stacking interactions in crystals.

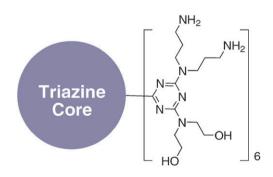


#### 1918

Polycationic triazine-based dendrimers: effect of peripheral groups on transfection efficiency

Meredith A. Mintzer, Olivia M. Merkel, Thomas Kissel\* and Eric E. Simanek\*

A small library of triazine dendrimers differing in the number and type of cationic groups with a variety of neutral groups has been screened for transfection efficiency and other physicochemical parameters.



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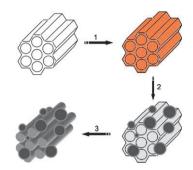
#### **PAPERS**



#### An easy co-casting method to synthesize mesostructured carbon composites with high magnetic separability and acid resistance

Limin Guo, Shaozhong Zeng, Jiangtian Li, Fangming Cui, Xiangzhi Cui, Wenbo Bu and Jianlin Shi\*

Magnetic mesoporous carbon composites were directly replicated from SBA-15 and the saturation magnetization value can be easily tuned. Furthermore, the composites show good acid resistance due to a carbon shell around the magnetic particles.

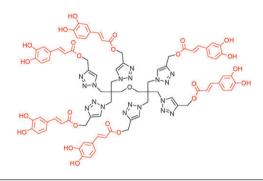


#### 1932

#### Caffeoyl and cinnamoyl clusters with anti-inflammatory and anti-cancer effects. Synthesis and structure-activity relationship

Luc H. Boudreau, Nadia Picot, Jérémie Doiron, Benoît Villebonnet, Marc E. Surette, Gilles A. Robichaud and Mohamed Touaibia\*

Novel caffeoyl and cinnamoyl clusters were prepared and their anti-inflammatory and anti-cancer effects were evaluated.



#### 1941

#### Tail-end amphiphilic dimethylaminopyridinium-containing polymethacrylates for gene delivery

Pascal Y. Vuillaume,\* Mélanie Brunelle, C. Géraldine Bazuin, Brian G. Talbot, André Bégin, Marie-Rose Van Calsteren and Sylvette Laurent-Lewandowski

Polyplexes obtained from Br-neutralized polyamphiphiles with the n = 12 spacer are efficient gene delivery agents.

#### 1951

#### Lactic acid-magnesium oxide nanocrystal interactions: how nanoparticle size and shape affect chemistry and template oligomerization

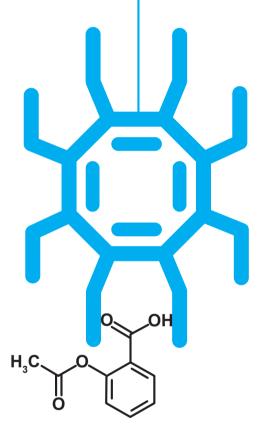
Erin M. Beavers, Kenneth J. Klabunde,\* Biobing Wang and Susan Sun

Starburst TEM images of polylactic acid templated by nanocrystals of magnesium oxide.





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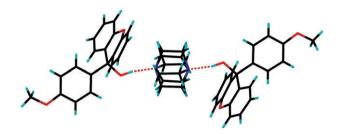


#### 1960

### Enclathration by a xanthenol host *via* solid–solid reactions: structures and kinetics

Ayesha Jacobs,\* Luigi R. Nassimbeni, Kanyisa L. Nohako, Gaelle Ramon and Jana H. Taljaard

The host compound 9-(4-methoxyphenyl)-9*H*-xanthen-9-ol forms an inclusion compound with triethylenediamine.



#### 1965

### Anthracene-based open and macrocyclic receptors in the flurometric detection of urea

Kumaresh Ghosh\* and Goutam Masanta

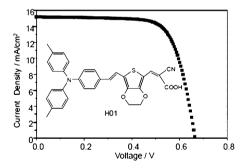
Anthracene-based open and macrocyclic receptors 1 and 2 have been designed and synthesized for the recognition of urea in less polar  $CHCl_3$  and more polar  $CH_3CN$  solvents. The receptor binds urea strongly in  $CHCl_3$  and exhibits a significant increase in the emission of the anthracene. Both receptors 1 and 2 are examples of PET sensors for the recognition of urea.

#### 1973

# A novel ruthenium-free TiO<sub>2</sub> sensitizer consisting of di-p-tolylaminophenyl ethylenedioxythiophene and cyanoacrylate groups

Ke-Jian Jiang, Kazuhiro Manseki, You-hai Yu, Naruhiko Masaki, Jiang-Bin Xia, Lian-Ming Yang, Yan-lin Song\* and Shozo Yanagida\*

A resource benign ruthenium-free organic dye was synthesized and employed as a sensitizer in DSCs with a high conversion efficiency of 7.33%.



#### **AUTHOR INDEX**

Ahamed, B. Nisar, 1825 Asokananthan Nithiananthan, 1869 Bazuin, C. Géraldine, 1941 Beavers, Erin M., 1951 Bégin, André, 1941 Bonnitcha, Paul D., 1845 Boudreau, Luc H., 1932 Brunelle, Mélanie, 1941 Bu, Wenbo, 1926 Caminade, Anne-Marie, 1809 Cano, Joan, 1901 Chaudret, Robin, 1833 Chechik, Victor, 1837 Colacio, Enrique, 1901 Cui, Fangming, 1926 Cui, Xiangzhi, 1926 Cysewski, Piotr, 1909 Dilworth, Jonathan R., 1845 Doiron, Jérémie, 1932 Esterbauer, Andreas J., 1829 Fairlamb, Ian J. S., 1837 Galletti, Paola, 1859 Ghosh, Kumaresh, 1965 Ghosh, Pradyut, 1825 Guillaume, Glemence, 1853 Guo, Limin, 1926 Han, Buxing, 1841 Hao, Erhong, 1888 Herrera, Juan Manuel, 1901 Holland, Jason P., 1845 Hurst, Eleanor C., 1837

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**Highlights in** 

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# **Chemical Science**

Dual function agents allow more control of radiopharmaceutical doses for cancer

Image is everything

Improved radiopharmaceutical agents to detect and treat cancer in bones have been developed by UK

Philip Blower and colleagues from King's College London and Barts and The London School of Medicine made a dual function molecule containing a bisphosphonate to target bones and a radio-labelled part to image in just two steps.

Cancer spreading from a tumour into bone, known as bone metastasis, is a common problem in cancer patients and can cause pain. Treatment involves injecting <sup>99m</sup>technetium or <sup>188/186</sup>rhenium bisphosphonates into the body. The bisphosphonates accumulate in the bone and treat the area and the radio-labelled metals aid imaging by single photon emission computed tomography. But technetium bisphosphonates exist as mixtures of compounds, making it difficult to establish each component's role, explains Blower. Rhenium complexes are easily degraded by

enzymes, leading to lower bone uptake and higher radiation doses in soft tissue, he adds. 'Our motivation was to reduce these effects so that doctors are more likely to prescribe this form of treatment,' explains Blower. 'We

would like ultimately to be able to give doses that are high enough not just to relieve pain but to treat the cancer and extend life expectancy.'

In current treatments, the bisphosphonates both chelate the metal and bind to bone. Blower separated the bisphosphonate and metal with a spacer, which bound strongly to the metal leaving the bisphosphonate free to perform just one role - targeting bone. The twostep synthesis is easy and results in single, well-defined complexes.

The molecule consists of a bisphosphonate bone-seeking agent and a radio-labelled part separated by a spacer

Reference

R Torres Martin de Rosales et al. Chem Commun. 2009. 4847 (DOI: 10.1039/b908652h)

'From a chemical perspective they're far superior to the agents we have already because we have a single compound and not a mixture of really unknown compounds,' says Blower of his molecules. 'and once we know what the chemistry is, it is under our control and we can optimise it and make it do what we want to do by changing the structure.'

'It's interesting that a single-molecule complex with bisphosphonates accumulates in the bone matrix as it is commonly maintained that only polymeric species can do this job,' says Adriano Duatti, an expert in molecular imaging at the University of Ferrara, Italy. 'A truly remarkable achievement would be to produce the corresponding <sup>188</sup>Re complex in high specific activity, as currently, there is no effective <sup>188</sup>Re agent for the treatment of bone metastases.' Ian Coates

### In this issue



### **Superhydrophobicity saves scalding**

Clothes coated with a Teflon-carbon nanotube composite could repel hot water

### Ice gels take the heat

A non-toxic scaffold for stem cell tissue engineering

### **Uranium chemistry: the final frontier**

New uranium compounds for the future of nuclear power

### **Bending the rules**

Guy Bertrand talks about creating dream compounds, tennis and setting up international labs in this month's interview









A snapshot of the latest developments from across the chemical sciences

# **Research highlights**

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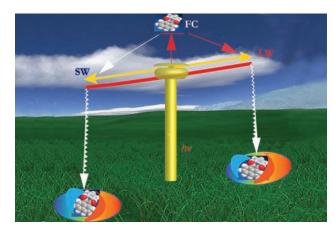
A seesaw helped scientists to discover dual fluorescent dyes

# Dyes get the green, and red, light

With the help of a photophysical model, scientists in the US have discovered dual fluorescent dyes (where two colours are emitted from the same fluorophore), which could prove useful in detecting clinically important molecules.

Michael Heagy and co-workers from the New Mexico Institute of Mining and Technology synthesised a matrix of nine naphthalimide dyes. They used a seesaw balanced photophysical model to balance the dyes' electronic properties by directing substituent groups on the dyes to the correct positions. Four out of the nine dyes in the matrix showed dual fluorescence.

Just as green and red traffic signals convey far more information to a motorist than a single yellow caution flasher, so also is the greater information obtained from dyes that emit in two colours to researchers who are attempting to detect a molecule, an ion or another clinically important system,' explains Heagy.



'The ability to obtain two colours from an organic dye improves biological analyses by providing a second signal or output to monitor. This enables better accuracy as the second colour provides internal calibration of the signal.'

Obtaining dual fluorescent dyes has previously proved difficult because of factors such as A seesaw model was used to balance the dyes' electronic properties by directing substituent groups on the dyes to the correct positions

#### Reference

P Nandhikonda *et al, Chem. Commun.*, 2009, 4941 (DOI: 10.1039/b911768g)

substituent groups on the molecule and the solvent affecting whether dual fluorescence will occur. Chemists have had to synthesise large libraries of dyes where only a small fraction turn out to be dual fluorescent.

Robert Strongin, who develops new organic reagents used in diagnosing, understanding and treating diseases at Portland State University, US, says, 'It's not often that simple and elegant predictive models for tuning fluorophore photophysics are reported.' He adds that the work of Heagy's group represents 'a breakthrough that will allow better understanding of fluorophore properties, and enable the design of improved optical materials.'

Heagy envisions dual fluorescent naphthalimide dyes being used in chemosensory devices for ion and molecule detection because of their advantages over conventional onecolour dyes. Fay Nolan-Neylan

Scientists have made new uranium compounds for the future of nuclear power

# **Uranium chemistry: the final frontier**

US scientists have synthesised complexes that could provide us with a new insight into the chemistry of uranium, with far reaching consequences for the nuclear industry and beyond.

Trevor Hayton and colleagues at the University of California, Santa Barbara, have made and isolated new uranium compounds containing an azide group, including uranium(v) azides. It is the first time, says Hayton, that uranium(v) azides have in fact been made. The team now hopes to harness the azide group's well-known reactivity to synthesise uranium nitride complexes.

Uranium nitride is a ceramic compound used as a nuclear fuel.
NASA is interested in using it as a future fuel for nuclear reactors used in space exploration. The compounds have also received attention recently as potential fuels for the next-generation of nuclear power systems.

Actinide nitrides are particularly promising as advanced nuclear fuels since they exhibit higher thermal conductivity and higher metal density compared with the oxides that are currently used.

Nitrides are a relatively rare functional group for uranium, says Hayton, and so few examples are available for scientists to study. He hopes, by using his new uranium azides, to carry out small-scale synthesis of uranium nitride and improve the understanding of its chemical properties. This would help scientists to predict its behaviour in nuclear waste and in the environment resulting in breakthroughs in waste processing and environmental

e for hopes.

Uranium azides could be used to make nitrides, which are particularly promising as advanced nuclear fuels remediation.

Uranium is also of great fundamental interest as it possesses chemical traits that are not found in any other element, says Hayton. These unique features may result in the development of novel catalytic reactivity. Many challenges remain in uranium chemistry and in actinide chemistry in general, adds Hayton, describing it as being 'the last frontier of the periodic table'.

Christopher Cummins, from the Massachusetts Institute of Technology, Cambridge, US, welcomes the work and says 'it elegantly unfurls a larger uranium(IV/V) coordination chemistry of azide as a nitrogen-rich pseudo-halide.'

Sarah Corcoran

#### Reference

S Fortier, G Wu and T W Hayton, Dalton Trans., 2010. DOI: 10.1039/b909879h

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### Clothes could repel hot water with a Teflon-carbon nanotube composite coating

# Superhydrophobicity saves scalding

A coating designed for clothing could help reduce industrial injuries due to scalding, say Chinese scientists.

Victims of hot water scalds often experience substantial burns as a result of the water wetting their clothing. 'The use of superhydrophobic textiles seems to be a promising way to protect the victims from deeper scalding,' says Yuyang Liu at The Hong Kong Polytechnic University and colleagues.

Superhydrophobic surfaces, such as Teflon and lotus leaves, exhibit high repellency to cool water. However, Liu and co-workers have discovered that a number of such surfaces show significantly reduced repellency to hot water. Their study led them to develop a fabric coated with a Teflon and carbon nanotube composite, which demonstrated promising repellency properties



A water droplet on a superhydrophobic surface

#### Reference

Y Liu, X Chen and J H Xin, *J. Mater. Chem.*, 2009, **19**, 5602
(DOI: 10.1039/b822168e)

to hot beverages including tea and coffee.

Liu's work quantified water repellency both in terms of the shape of droplets placed on the surface (static water) and the ability of sprayed droplets (dynamic water) to slide off the surface. While a standard Teflon-coated fabric scores well with regards to static water, its response to dynamic water is poor. Liu's material aimed to rectify this by using carbon nanotubes to increase the surface roughness, which improves superhydrophobicity by trapping air bubbles in tiny pores.

It is possible that the smaller length scale associated with the carbon nanotubes means that the superhydrophobic surface effect can withstand higher water impact pressures,' suggests Glen McHale of Nottingham Trent University, UK, who studies superhydrophobic surfaces. He warns that 'further work would be needed to repeat these tests and verify the mechanism.' Liu acknowledges that 'the creation of superhydrophobic surfaces which can repel pressured hot liquids is still a great challenge to scientists.' Erica Wise

### Scientists have made a non-toxic scaffold for stem cell tissue engineering

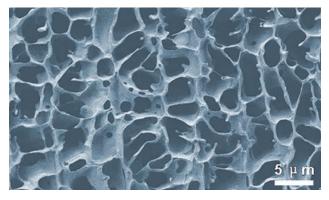
# Ice gels take the heat

Chinese scientists have combined two separate scaffold-making techniques to create an artificial biomaterial that can withstand conditions in the body.

Biomaterials are materials designed to replace or improve a natural function of a living structure. These materials can either be natural or man-made.

Xiang Yao from Tsinghua University, Beijing, and colleagues combined ice-segregationinduced self-assembly (ISISA) and electrostatic self-assembly (ESA) to fabricate macroscale biomaterials from nanoscale building blocks.

In ISISA, ice is used as a template to fabricate a porous structure whereas ESA uses two oppositely charged particles, suspended in a fluid, to attract each other. The ESA process has mainly been used to make 2D biomaterials, but Yao says his goal was 'to achieve a three dimensional and nanometre level biomimetic control of cell behaviour.' ISISA has been used to create 3D scaffolds but because the scaffolds are held



The 3D biocompatible structures were grown on ice

#### Reference

X Yao, H Yao and Y Li, *J. Mater.* Chem., 2009, DOI: 10.1039/ b909059b together with weak forces with this method, a water soluble polymer such as polyvinyl alcohol is often used to bind them together. Unfortunately, the polymer is toxic, which limits its use in tissue engineering.

When Yao combined the two methods by using ESA building blocks in an ISISA process, the team found that the resulting 3D scaffold was strong in water at 37 °C without the need to add toxic binders. This makes it suitable for use

in physiological environments and Yao says he hopes his research can be used in biomedical applications such as stem cell tissue engineering.

'The absence of crosslinkers should improve their biocompatibility as biomaterials but this issue must still be addressed,' says Marisa Ferrer, an expert in biomaterial design and application at the Instituto de Ciencia de Materiales de Madrid, Spain, who adds: 'The combination of ice ISISA and ESA beats the challenge of preparing 3D scaffolds working at physiological pH.'

Paul Hatton, who works on tissue engineering and polymer biocompatibility at the University of Sheffield, UK, comments that Yao's work is 'an elegant solution to one of the more significant challenges faced by those seeking to fabricate biomimetic materials, that of how to "build in" a nanoscale level of hierarchy in order to contribute to functional properties.' Rebecca Brodie

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### Simplified DNA logic gates detect biomarkers

# A logical extension

DNA logic gates can now detect more than just DNA segments, and by exploiting nature's design, their preparation could be simpler than ever.

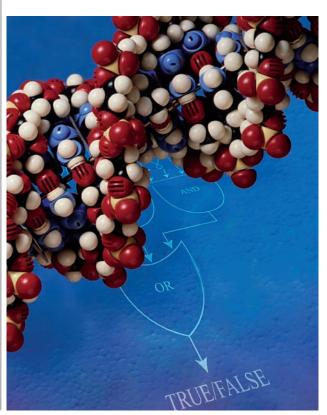
Atsushi Ogawa and Mizuo Maeda from The Institute of Physical and Chemical Research (RIKEN), Saitama, and Ehime University, Japan, have developed existing DNA logic gate systems to create a detection system where gold nanoparticle aggregation provides a visual marker for a variety of biomarkers.

Logic gates are used in digital circuits in computer chips. An input signal goes through a binary operation to give either a true (one) or false (zero) output. This system has been mimicked in biology using DNA inputs, outputs and switches. DNA logic gates detect oligonucleotides (short DNA segments) when they bind to the logic gate sensors. This concept has been developed to detect different molecules using aptamers-DNA or RNA molecules adapted to

#### Reference

A Ogawa and M Maeda, Chem. Commun., 2009, DOI: 10.1039/ h910288d

A true or false output that can be monitored by eye is given by the DNA logic gates



bind to other molecules and viruses. However, both DNA and aptamer logic gates have a drawback in that they rely on a hybridisation switch. When a target molecule binds, or hybridizes, to the sensor, the event has to be transmitted to a reporter system, which must be specifically engineered for each sensor/target

To avoid the need to design a hybridisation switch, Ogawa and Maeda based their logic gate on a cleavase aptazyme. An aptazyme is an enzyme which naturally produces a response upon interaction with a specific target or marker molecule. The aptazyme can be adapted to respond to virtually any species of interest, from a single ion, to a drug metabolite, which could have implications for medical diagnostic techniques. In this case, when activated by its target molecule, the cleavase aptazyme cleaves a length RNA from its own structure. The resulting free RNA transmits a signal to a reporter system: in this case. the pair used gold nanoparticles as reporters. They functionalised them with DNA strands that bind to the free RNA to form a duplex with a blunt end (where the ends of both strands are even rather than one strand being longer than the other). The duplexes facilitate nanoparticle aggregation, which can be seen with the naked eye by clearing of an otherwise cloudy reaction medium.

'We want to apply this method to construct more complex logic gates,' says Ogawa. 'Because the aggregation of gold nanoparticles depends on whether or not DNA on the nanoparticles forms a duplex with the cleaved RNA with a blunt end, we think an appropriate design of the cleaved RNA sequences may make them possible.'

Milan Stojanovic, an expert in diagnostic molecular devices based on nucleic acids, at Columbia University, New York, US, says that the work is an 'important contribution' towards a field that 'has a future if it moves in the direction of autonomous therapeutic devices, rather than towards competing with silicon.' Katie Dryden-Holt

### **News in brief**

This month in Highlights in **Chemical Technology** 

#### Nanoparticles take on terrorism

Tiny amounts of explosives such as TNT can be detected

#### Sterile surfaces in a flash

European scientists have created light-activated antimicrobial surfaces by modifying a material used in medical devices with tiny amounts of commonly used dyes.

#### **C**orn waste converted to chemicals

Biofuel waste could be turned into building blocks for industrial chemicals.

#### **Holography speaks volumes**

Søren Hvilsted discusses how holograms could be the answer to the increasing demand for data storage

#### **Raising the bar**

In this month's interview, Scott Tanner talks about measuring cell biomarkers and Olympic gymastics

See www.rsc.org/highlightschemtech for full versions of these articles

This month in Highlights in **Chemical Biology** 

#### Nano-earthquake to shake up drug screening

A thumbnail-sized chip mimics the turbulent conditions a drug experiences on its journey through the body

#### **Blood cells get active**

A cell boosting peptide could help diabetics

#### **Untangling Alzheimer's**

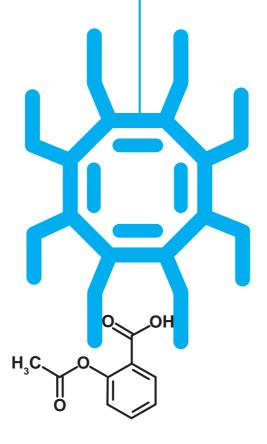
Cures for Alzheimer's may come from understanding its chemistry. Arvi Rauk examines the disease at the molecular level

#### **Genetic alphabets**

In this month's interview, Ichiro Hirao talks about nucleic acid research, expanding the genetic code and the possibility of creating new life.

See www.rsc.org/highlightschembiol for full versions of these articles

# New adventures on the web



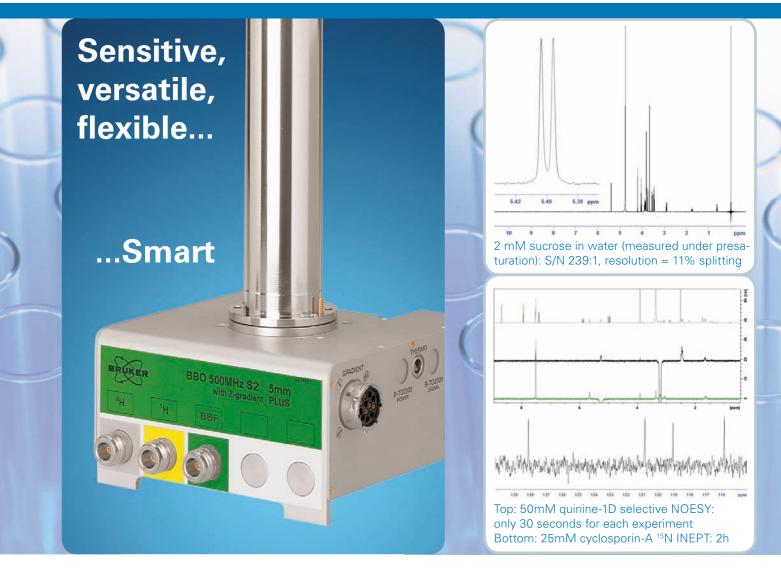
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# **Interview**

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# **Bending the rules**

Guy Bertrand talks to Marie Cote about creating dream compounds, tennis and setting up international labs



#### **Guy Bertrand**

**Guy Bertrand is a Distinguished Professor of Chemistry at** the University of California, Riverside (UCR), CA, US, where he heads the UCR/CNRS (National Center for Scientific Research) joint laboratory. His research interests concern main group elements and are at the interface between organic, organometallic and inorganic chemistry. Major ongoing projects in Guy Bertrand's group are the synthesis of stable carbenes, highly reactive intermediates and defying standard valence rules.

#### What led you to chemistry?

I do not think I was programmed to become a chemist. I wanted to be a tennis player, but I was better at school than on the court! Then, I studied science. I did not like mathematics and physics, and at that time I found biology too empirical, so I chose chemistry.

#### Where do you look for ideas?

All along my career, I have tried to demonstrate that some of the rules we learned at school are not totally correct, or at least that we can find tricks to get around them. A good illustration is given by our recent synthesis of push–push allenes, which are flexible and bent, whereas regular allenes were believed to be rigid and linear. Do not misunderstand, I am a deep admirer of ancient chemists who were working without the modern technological tools, and this is my way to render homage to them. In many of my papers there is a reference to a work from the beginning of the 20th century, or even earlier.

#### What is the most significant aspect of your work?

I guess that the synthesis of the first stable carbene in 1988 is the most important result of my career. At that time, very few chemists believed that carbenes could be isolated. Certainly nobody thought, including myself, that some twenty years later, carbenes would be ubiquitous ligands for transition metal based catalysts, and catalysts in their own right. Having said that, I have to recognise that our first stable carbene did not find applications by itself, and that the popularity of carbenes is mainly due to the so-called *N*-heterocyclic carbenes, discovered by my friend Bo Arduengo. This perfectly illustrates that it is difficult to predict if a discovery, as spectacular as it is, will be important for the future or not.

When we found stable diradicals, we thought that ourselves, or somebody else, would quickly find applications for them in materials science. So far, this has not been the case and diradicals are still laboratory curiosities! The future will also tell us if cyclic bent-allenes, which we have recently described, are important or not. Right now, I am quite optimistic. In any case, the most significant aspect of my work is hopefully what we will discover tomorrow!

#### What do you love about your job?

I can spend hours at the NMR or X-ray machine to be sure that we have really created the new chemical object we were dreaming of. The success of former PhD students or postdoctoral fellows is also very rewarding. To make a comparison, when I was young I played tennis, and I wanted to be the best; now I am more interested to see my kids winning a game, than winning a game by myself.

### You are a keen communicator. How would you define the importance of teaching?

In the US, the barrier between the professors and the students is almost non-existent, and I like it. My aim here is to make chemistry as attractive as possible for every student. My great pleasure is to see some of the students majoring in biology change their mind and become chemistry majors!

# Having worked both in Europe and in the US, what would you say the major differences are in the life of an academic?

To begin an academic career, I am quite convinced that the US system is better, although very brutal. For all scientists, it is more stressful to work in the US, especially at a time when the budgets are tight, but I find this very exciting and stimulating. However, to increase your chance of funding, you need to work in a 'fashionable area', and to demonstrate that your research will quickly find applications. This is an extremely important aspect, since most of the time practical applications of a fundamental discovery occur years afterwards. Lastly, there is the existence of a strong competition between the US universities, and that makes the faculty of a department a real team. I would advise young scientists to test both, via postdoctoral stays abroad. Then, they could choose the one that suits them best.

# You point out that your laboratory is a joint venture between the University of California and the French CNRS. Can you comment on the collaboration?

I am very proud of this, and I believe that this is representative of the structure of fundamental research in the future. Globalisation is not only a word, it is a reality that we cannot ignore. I am quite confident that other agencies all over the world will follow and that many international labs will be created.

### Finally, what would be your message to the younger generation?

A very simple but very important one: science and scientists are not boring! We travel all around the world, meet new friends at conferences, and what can be more exciting than to make a tiny contribution to improving the welfare of humanity.

# **Essential elements**

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# **IUPAC 2009**

The RSC hosted the 42nd IUPAC Congress at the SECC, Glasgow, UK, and enjoyed meeting over 2000 delegates from 72 countries and 64 chemical societies. The programme featured seven themes: Analysis & Detection, Chemistry for Health, Education & Communication, Industry & Innovation, Materials, and Synthesis & Mechanism. RSC journals sponsored a variety of sessions within the 50 symposia taking place. Speakers presented key research topics demonstrating the impact of the chemical sciences, and highlighting exciting innovations with an overall focus on 'Chemistry Solutions'.

Following the RSC's acquisition of ChemSpider, Graham McCann, Business Manager for ChemSpider,

joined Antony Williams, ChemSpider Vice President of Strategic Development, on the ChemSpider stand to share future plans on what the collaboration will bring to scientists. The new website, demonstrated on the stand, gave delegates

the opportunity to navigate around the website to see the new functionality it offers to users.

The RSC stand was

also very well attended. and showcased hot new titles including the very latest news on Analytical Methods and Nanoscale, the new journals to be launched later this year, and Polymer Chemistry, a new journal for 2010.

This year's IUPAC conference also saw the successful launch of RSC's highly interactive social networking tool, MyRSC.

> MyRSC allows chemical scientists to network with one another across the globe, share information about

> > themselves and their

research, receive details of career opportunities and join specialist groups. Visit http://my.rsc.org for the very latest information on this exciting new development, and to find out details on how to join. Don't miss out on the next **IUPAC** Congress in Puerto Rico in 2011! (www.iupac2011.org)

There are many other ways in

which technology has facilitated

international networking and

scientific advances. Gone are

the days when a researcher

waited for a print journal to

arrive on the desk to see the

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the occasional overseas trip to a

scientific conference to catch up

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overcome some of the global

scientists? We'd like to think so.

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dissemination of the latest

### **ChemSpider** sensation

August marks a milestone in ChemSpider's 2009 calendar. Just two months after announcing RSC's new partnership, we unveiled to the world at the 42nd IUPAC Congress in Glasgow a refreshed looking ChemSpider, now hosted on powerful RSC servers.

The ChemSpider booth at the event was abuzz: delegates searched for chemicals they didn't expect ChemSpider to have ... and found them! They deposited and curated data live. People who'd never heard of ChemSpider rushed to tell others. We heard comments like, 'This is the best thing I have seen all day' and 'Do you realise how much this will do for the world of chemistry?

Delegates were impressed by the fast text and structure searching capabilities, the size and diversity of the database (including videos, reactions and blog posts). They were also complimentary about the new ChemSpider look and feel delivered through the logo, exhibition booth and literature, and excited about ChemSpider's vision for the future.

The ChemSpider team thanks everyone for their support.

Search, share and help refine the data at www.chemspider.com



### **Working together**

What do a free online source of structure-based chemical information, Twitter and a roadmap have in common?

They are all ways in which the RSC is working with the global scientific community - and they all feature in Issue 2, 2009 of Fusion, RSC Publishing's newsletter, which has a distinct technology theme. We, as members of the community, have a vast range of new and emerging technologies at our disposal. We can alert you to an article immediately it is published online, and provide links to open online resources to help you enhance your knowledge.



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