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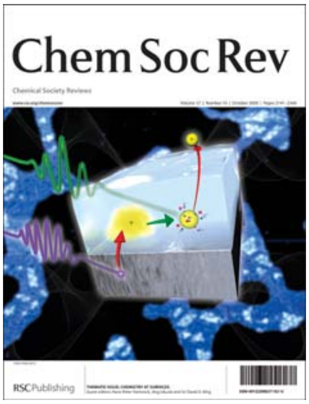
IN THIS ISSUE

ISSN 0306–0012 CODEN CSRVBR 37(10) 2141–2360 (2008)



Cover
Light-induced elementary processes at ice–metal interfaces are probed by femtosecond two-photon photoemission; interface structure is analyzed by STM (background by K. Morgenstern and co-workers, Leibniz Universität Hannover, Germany). Image reproduced by permission of Julia Stähler, Uwe Bovensiepen, Michael Meyer and Martin Wolf from *Chem. Soc. Rev.*, 2008, **37**, 2180.

Inside Cover
See Oliver R. Inderwildi and Stephen J. Jenkins, page 2274. Catalytic combustion and synthesis of hydrocarbons, classic reactions reassessed here ***via*** modern computational theory, could underpin an efficient "carbon cycle" for sustainable biofuel exploitation. Image reproduced by permission of Oliver R. Inderwildi and Stephen J. Jenkins from *Chem. Soc. Rev.*, 2008, **37**, 2274.

CHEMICAL SCIENCE

C73

Drawing together research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences, showcasing newsworthy articles and significant scientific advances.

Chemical Science

October 2008/Volume 5/Issue 10

www.rsc.org/chemicalscience

EDITORIAL

2153

Chemistry at surfaces

Hans-Peter Steinrück, Jörg Libuda and Sir David A. King

Guest editors Hans-Peter Steinrück, Jörg Libuda and Sir David A. King introduce this thematic issue of *Chemical Society Reviews* covering reactions at surfaces in honour of the 2007 Nobel Prize winner Professor Gerhard Ertl. Photo credit: Wolfram Däumel - Fritz-Haber-Institut der Max-Planck-Gesellschaft.

Gerhard Ertl

Chem Soc Rev

Chemical Society Reviews

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Chemical Society Reviews publishes accessible, succinct and reader-friendly articles on topics of current interest in the chemical sciences. The promotion of international and multidisciplinary awareness and cooperation is particularly encouraged. Chemical Society Reviews publishes two article types: tutorial reviews, which present an accessible introduction to the topic, and critical reviews, which provide a deeper evaluation of the current literature.

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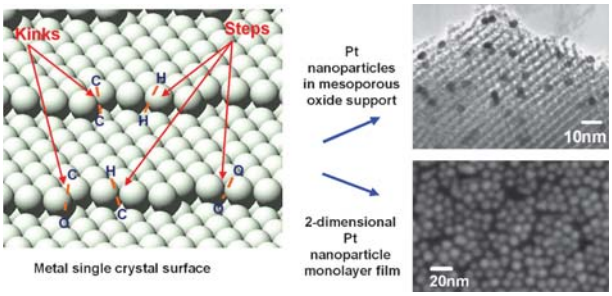
2155

Molecular surface chemistry by metal single crystals and nanoparticles from vacuum to high pressure

Gabor A. Somorjai* and Jeong Y. Park

The evolution of the model systems for the study of molecular chemistry and catalysis by surfaces from single crystals to colloid nanoparticles under high pressure is highlighted in this review.

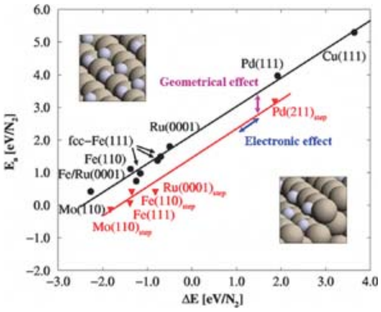


2163

The nature of the active site in heterogeneous metal catalysis

Jens K. Nørskov,* Thomas Bligaard, Britt Hvolbæk, Frank Abild-Pedersen, Ib Chorkendorff and Claus H. Christensen

We present a partitioning of geometrical and electronic effects in heterogeneous catalysis and define the concept "degree of structure sensitivity".

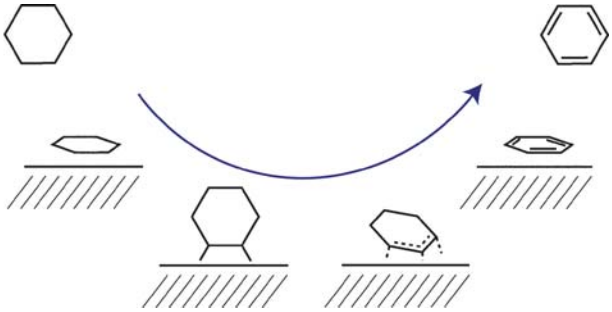


2172

Catalytic reaction energetics by single crystal adsorption calorimetry: hydrocarbons on Pt(111)

Ole Lytken, Wanda Lew and Charles T. Campbell*

Recent advances in single crystal adsorption calorimetry are reviewed, using selected studies of adsorption and dehydrogenation of hydrocarbons on Pt(111).

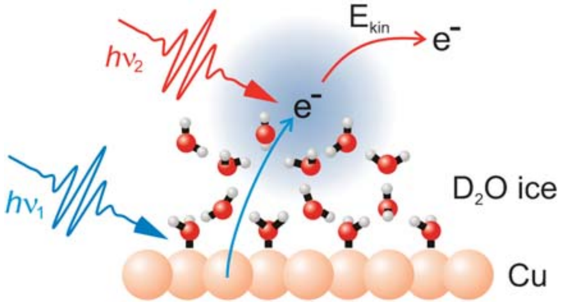


2180

A surface science approach to ultrafast electron transfer and solvation dynamics at interfaces

Julia Stähler, Uwe Bovensiepen, Michael Meyer and Martin Wolf

Time-resolved photoelectron spectroscopy provides detailed insights into interfacial electron transfer and solvation dynamics at ultrathin ice layers on metal surfaces.



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Soft Matter

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Soft matter is not a new topic - indeed de Gennes was awarded a Nobel prize for research into soft matter in 1991. However more and more researchers are realising that the work they do, on the edges of physics, chemistry, materials science, or biology, does not fit into these traditional disciplines but it does fit under the umbrella term of 'soft matter'.

This meeting aims to give researchers from all areas of soft matter the chance to discuss their research and to see how their knowledge can be applied in solving a range of soft matter problems, from adhesion to cell membranes to rheology of polymer mixtures.

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- Proteins and cells (e.g. cell adhesion, membranes, biophysics)
- Surfaces/rheology (e.g. polymer physics, theory)

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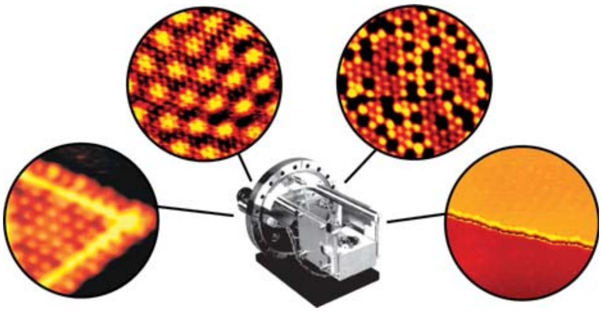
TUTORIAL REVIEWS

2191

Scanning tunneling microscopy as a tool to study catalytically relevant model systems

Ronnie T. Vang, Jeppe V. Lauritsen, Erik Lægsgaard and Flemming Besenbacher*

STM is a unique tool for the study of surface processes on model systems relevant to heterogeneous catalysis.

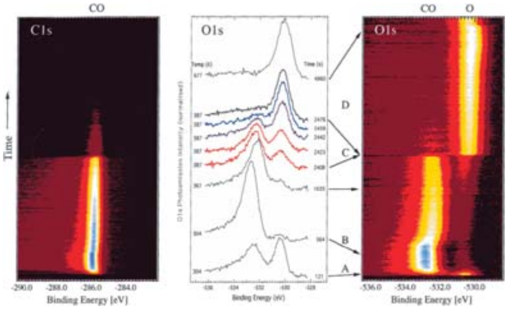


2204

Automotive catalysis studied by surface science

Michael Bowker

Surface science enables researchers to 'see' reactions at surfaces and to resolve catalytic phenomena.

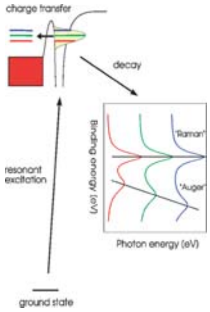


2212

Ultrafast charge transfer at surfaces accessed by core electron spectroscopies

Dietrich Menzel

The use of the short lifetimes of core holes (~0.1 to 10 fs) to clock ultrafast charge transfer between adsorbates and substrates is described and exemplified.



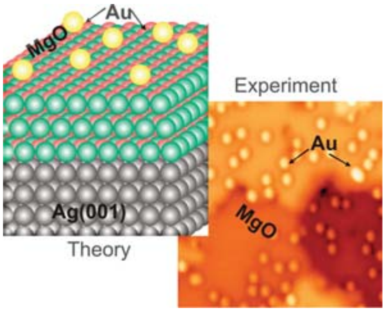
CRITICAL REVIEW

2224

Oxide ultra-thin films on metals: new materials for the design of supported metal catalysts

Hans-Joachim Freund and Gianfranco Pacchioni

Oxide ultra-thin films on metals not only provide good models of supported metal catalysts, but can exhibit new properties with no counterpart in bulk oxides.



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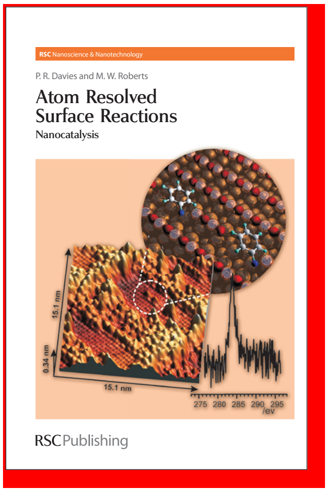
Atom Resolved Surface Reactions: Nanocatalysis

Authors: P R Davies and M W Roberts


RSC Nanoscience & Nanotechnology

P. R. Davies and M. W. Roberts

Atom Resolved Surface Reactions

Nanocatalysis

RSC Publishing

This book offers a unique perspective of the impact of scanning probe microscopies on our understanding of the chemistry of the surface at the nanoscale. Topics discussed include:

- The dynamics of oxygen chemisorption at metal surfaces
- Control of oxygen states and surface reconstruction
- Dissociative chemisorption of diatomic and hydrocarbon molecules
- Nanoparticles and chemical reactivity
- STM at high pressures
- Structural studies of sulfur containing molecules and molecular templating

Ideal for those who wish to become familiar with the contribution Scanning Tunnelling Microscopy has made to the understanding of the field of surface chemistry and heterogeneous catalysis and also to those who are new to catalysis, a fascinating and important area of chemistry!

BB Hardback | xviii + 222 pages | ISBN 9780854042692 | 2007 | £90.00

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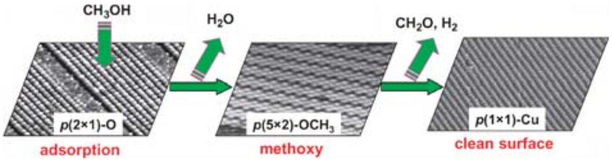
CRITICAL REVIEWS

2243

Unraveling molecular transformations on surfaces: a critical comparison of oxidation reactions on coinage metals

Xiaoying Liu, Robert J. Madix* and Cynthia M. Friend

Current state of molecular-level knowledge is reviewed for oxidation of alcohols and olefins on coinage metals, copper, silver, and gold.

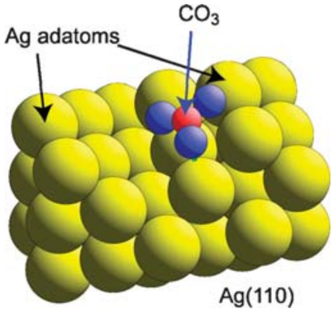


2262

The local structure of molecular reaction intermediates at surfaces

D. P. Woodruff

The detailed bonding geometry of chemical reaction intermediates on surfaces is now known for a number of systems.

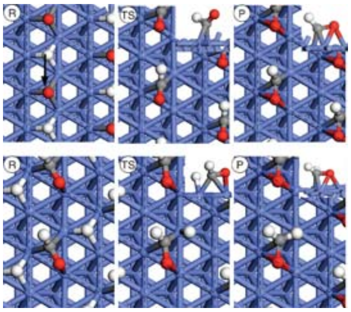


2274

In-silico investigations in heterogeneous catalysis—combustion and synthesis of small alkanes

Oliver R. Inderwildi and Stephen J. Jenkins*

First-principles density functional calculations relevant to alkane oxidation and synthesis over transition metal catalysts are reviewed.

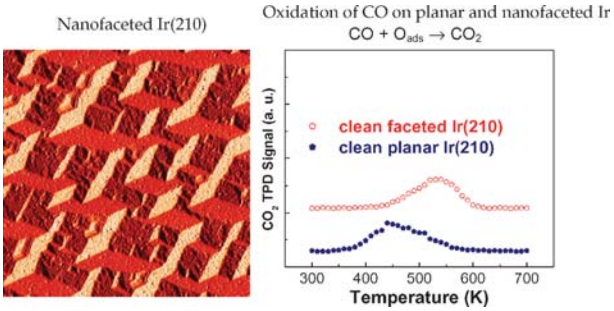


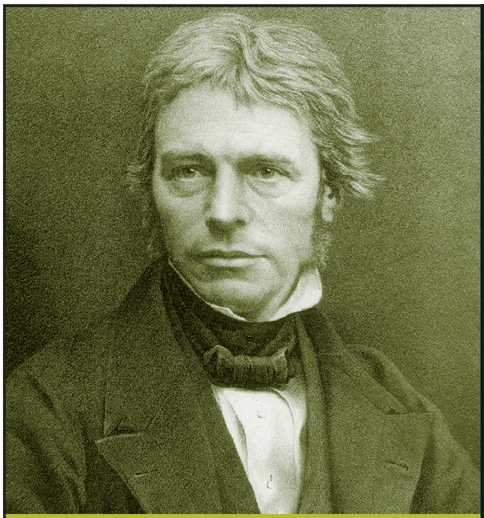
2310

Nanoscale surface chemistry over faceted substrates: structure, reactivity and nanotemplates

Theodore E. Madey,* Wenhua Chen, Hao Wang, Payam Kaghazchi and Timo Jacob*

Faceting occurs when an initially planar surface converts to a ‘‘hill and valley’’ structure, exposing new crystal faces of nanometre-scale dimensions. In this critical review we give an overview of the physics and chemistry of facet nucleation and growth on a variety of metal, semiconductor and oxide surfaces.





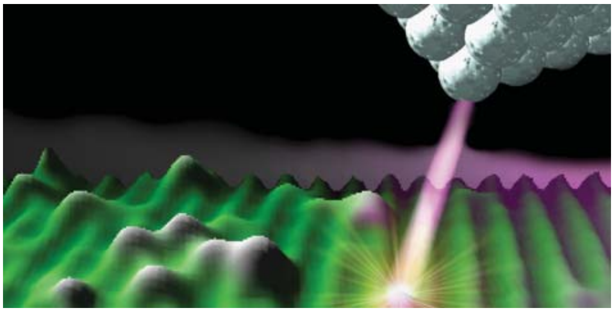
CRITICAL REVIEW

2328

Chemical reactions on rutile TiO_2(110)

Chi Lun Pang, Robert Lindsay and Geoff Thornton*

Understanding the surface chemistry of titania on the atomic scale.



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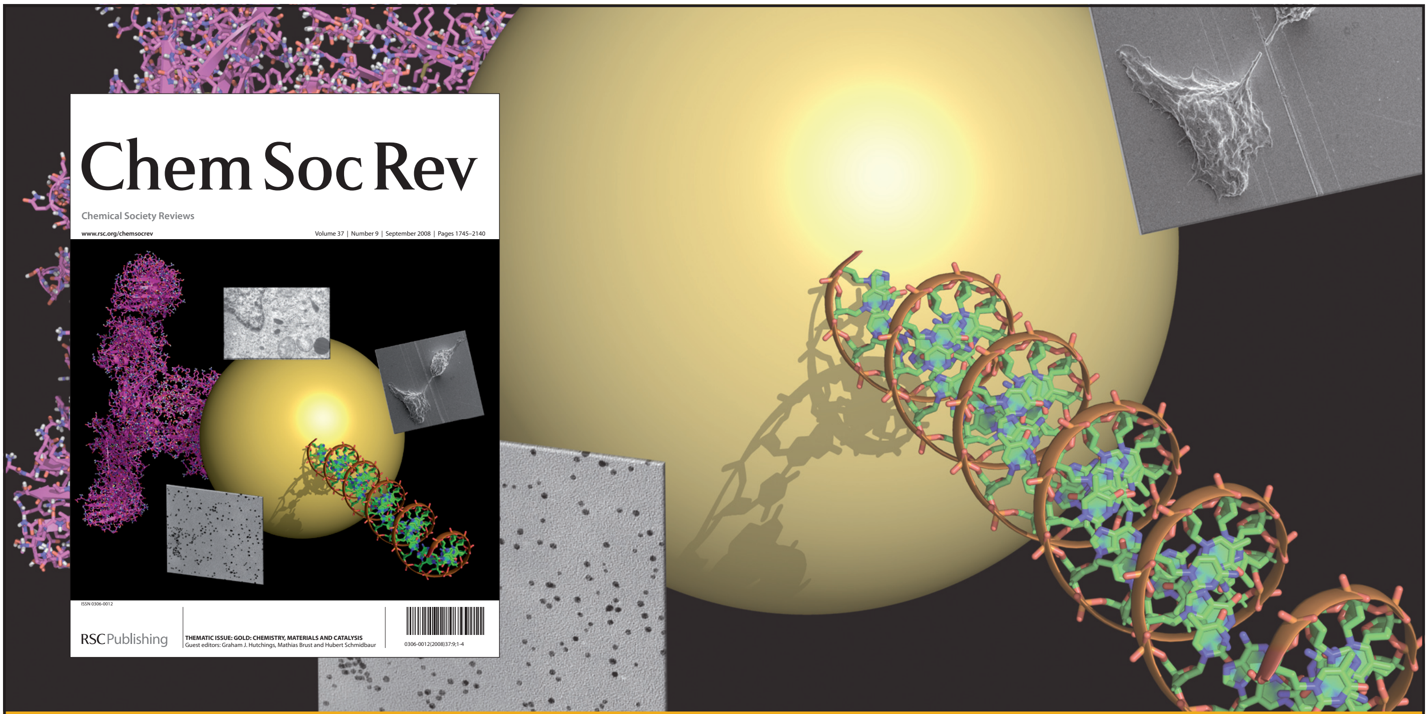

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ISSN 0306-0012

RSC Publishing

THEMATIC ISSUE: GOLD: CHEMISTRY, MATERIALS AND CATALYSIS
Guest editors: Graham J. Hutchings, Mathias Brust and Hubert Schmidbaur

0306-0012(2008)37:9;1-4

Gold: Chemistry, Materials and Catalysis theme issue

This collection of reviews sets out the state of the art with respect to gold catalysis, the synthesis and application of gold nanoparticles and gold chemistry. As such the issue takes a very broad approach to the topic, which has now become a hot topic in chemistry as a whole. We hope the reviews will inspire new discoveries and new researchers into this exciting field. The issue is timely as the field is expanding rapidly and hence these articles allow us to take stock of the great progress already achieved, as well as highlighting the remaining challenges.

Reviews include:

The relevance of shape and size of Au_{55} clusters
Günter Schmid

The chemistry of gold as an anion
Martin Jansen

Catalytically active gold on ordered titania supports
Mingshu Chen and D. Wayne Goodman

Biological applications of gold nanoparticles
Ralph A. Sperling, Pilar Rivera Gil, Feng Zhang, Marco Zanella and Wolfgang J. Parak

Shape control in gold nanoparticle synthesis
Marek Grzelczak, Jorge Pérez-Juste, Paul Mulvaney and Luis M. Liz-Marzán

The use of aurophilic and other metal–metal interactions as crystal engineering design elements to increase structural dimensionality
Michael J. Katz, Ken Sakai and Daniel B. Leznoff

Supported gold nanoparticles as catalysts for organic reactions
Avelino Corma and Hermenegildo Garcia

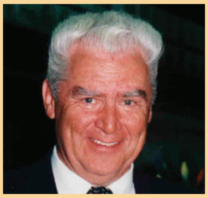
Guest editor

Graham J Hutchings
Cardiff University

Guest editor

Matthias Brust
University of Liverpool

Guest editor



Hubert Schmidbaur
Technische Universität München

'Catalysis is reaching a golden age, as gold is finding many new applications as a catalyst for selective oxidations and hydrogenations. It is a really exciting time to be working in the field of catalysis'

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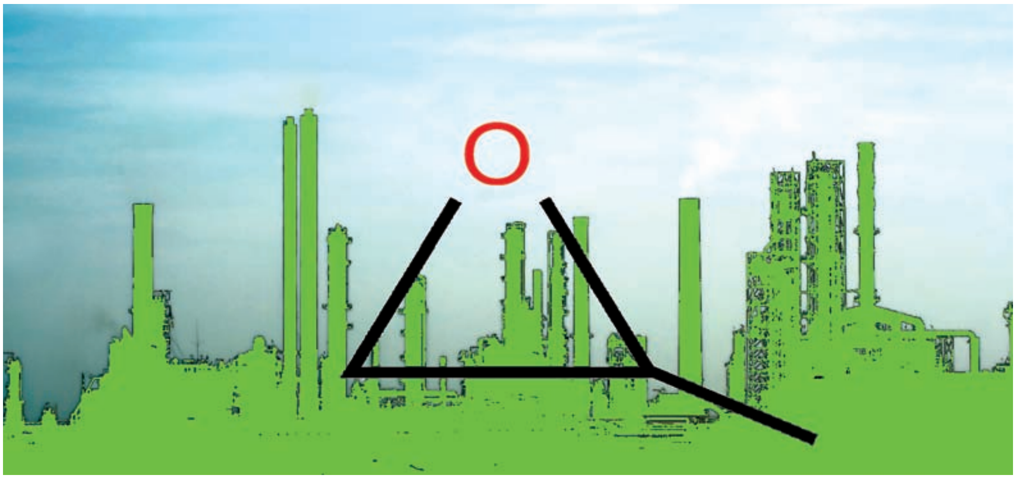
October 2008 / Volume 5 / Issue 10 / ISSN 1478-6524 / CSHCBM / www.rsc.org/chemicalscience

Chemical Science

An environmentally-friendly route to an industrial chemical is unveiled

Propylene oxide gets a green makeover



US chemists have developed a greener, higher yielding and more selective route to propylene oxide, an important industrial chemical that is manufactured worldwide on a million tonne scale.

Propylene oxide is a vital building block for making many other compounds and materials, such as surfactants and foams. However, the two routes used to manufacture it in bulk involve environmentally unfriendly peroxides and chlorinated materials to oxidise propylene, and produce undesirable waste products.

Qunlai Chen and Eric Beckman at the University of Pittsburgh have devised a one-pot route that uses a titanium-modified zeolite catalyst to prepare the oxidant hydrogen peroxide in situ from hydrogen and oxygen. Additionally the reaction solvent is environmentally benign liquid- or supercritical-carbon dioxide containing small quantities of methanol and water.

According to Beckman, many of the common side reactions of the process (such as propylene hydrogenation or propylene oxide hydrolysis) can be effectively suppressed by using an ammonium acetate additive to neutralise the surface acidity of the catalyst.

Propylene conversion rates are normally limited to less than 10% in order to maintain the required product selectivity. Using the one-pot route, Beckman obtains yields of over 21% with an 82% selectivity for the first time.

Propylene oxide is manufactured annually on a million tonne scale

Yasutaka Ishii, an expert in hydrocarbon oxidation reactions using hydrogen peroxide, based at Kansai University, Osaka, Japan, considers this method to be a very interesting green route for making propylene oxide, pointing out that no harmful waste is produced.

David Parker

Reference

Q Chen and E J Beckman, *Green Chem.*, 2008, **10**, 934 (DOI: 10.1039/b803847c)

In this issue

Sweet smell of success

Ionic liquids assist the synthesis of a lemon scented chemical

Natural product hybrids fight cancer

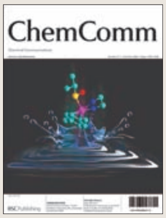
A potent hybrid of two anticancer natural products has been designed and synthesised

Instant insight: Lovely bubbly

Gérard Liger-Belair, University of Reims Champagne-Ardenne, France, celebrates what gives champagne its sparkle

Instant insight: Tasting the chemistry

Susan Ebeler, University of California, Davis, US, reveals the science behind the flavour in everyone's favourite tipple

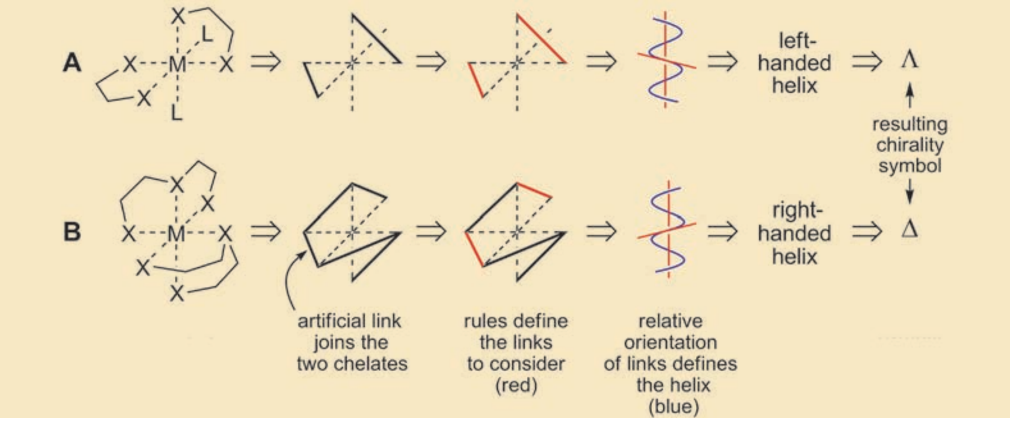


A snapshot of the latest developments from across the chemical sciences

Research highlights

A new proposal for defining the chirality of octahedral complexes is put forward

Getting to grips with complex chirality



Naming inorganic compounds is usually a routine operation, but one problem has long defied solution – how to define the chirality of certain octahedral complexes containing chelates (ligands with more than one point of attachment). Santiago Herrero from the Complutense University of Madrid, Spain, and his colleague have now proposed a way of doing this.

The general idea when defining the chirality of such complexes is to ignore the identity of the donor atoms on the ligands and any chiral centres on the chelates, as this can be dealt with by standard stereochemical symbols. Instead, the focus is the topology of the chelate network. This is how the six atoms attached to the central metal atom – the vertices of the octahedron – are joined together. The chelates are first drawn as straight lines joining the vertices. These lines are then compared, and the complex assigned as Λ(lambda) if they define a left-handed helix, and Δ (delta) if they define a right-handed helix. This is fine in simple complexes such as **A** (see image), but things get difficult in cases like **B**, because there is more than one possible pair of lines to compare. Herrero and Usón have now devised a heirarchy of rules that enable such systems to be dealt with.

The new system works by first (if necessary) artificially linking the chelates together so that the resulting line has the greatest number of changes of plane. A set of rules then allows you to pick a pair of links that you can use to define the complex as Δ or Λ. Further rules, involving consideration of all the vertices that are not directly joined, allow the designation of chirality in even stranger complexes.

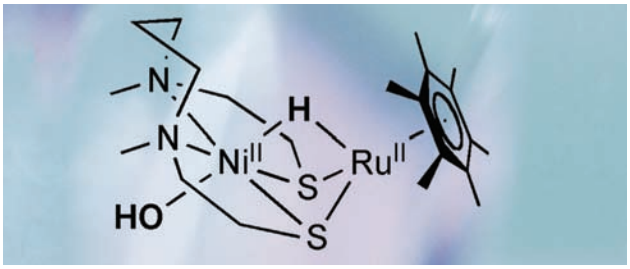
Defining the chirality of chelate-containing complexes is a long-standing problem

Although the chirality symbols in several cases are different under the new system, says Herrero, there are fewer rules to contend with. In conclusion, he says that their method 'could be useful for keeping and searching precise structural information about octahedral compounds'.
David Barden

Reference
S Herrero and M A Usón, *Dalton Trans*, 2008, 4993 (DOI: 10.1039/b806050a)

Water-soluble organometallics may aid the development of new types of catalysts

Energy from model enzymes



Mimicking enzymes with inorganic complexes could offer a new route to catalysing hydrogen fuel cells, claim Japanese scientists.

In nature, hydrogenases are enzymes that catalyse the splitting of hydrogen in its H_2 form into two separate protons and two electrons. However, there has been some controversy over the mechanism by which the enzyme operates, with mechanistic studies contradicting experimental data. Now, a group led by Seiji Ogo at Kyushu University, Fukuoka, have solved this problem by making a nickel-ruthenium complex that acts as a model of the enzyme. They say this complex could be used to develop new cathode catalysts for hydrogen fuel cells.

Described by Chris Pickett, an energy expert from University of East Anglia, Norwich, UK, as 'an elegant chemical precedent', the complex is water-soluble like natural hydrogenases, and so allows the first study of a model in the hydrogenases' natural environment.

Ogo explains that that understanding the exact mechanism of the hydrogenase will allow scientists to progress research into new types of catalysts for hydrogen fuel cells. The group studied how the complex reacts and showed that the generation of single and double exchange products is simultaneous, just as observed for the naturally occurring enzymes. Ogo is now looking forward to further studies on this model that should uncover more details of the reaction.

Impersonating nature could offer access to new types of catalysts for fuel cells

Water soluble organometallics like these have become more and more interesting for both life and materials sciences. Ogo hopes that technology for the extraction of electrons from hydrogen, using his new complexes can now be developed. *Laura Howes*

Reference
B Kure *et al*, *Dalton Trans.*, 2008, 4747 (DOI: 10.1039/b807555g)

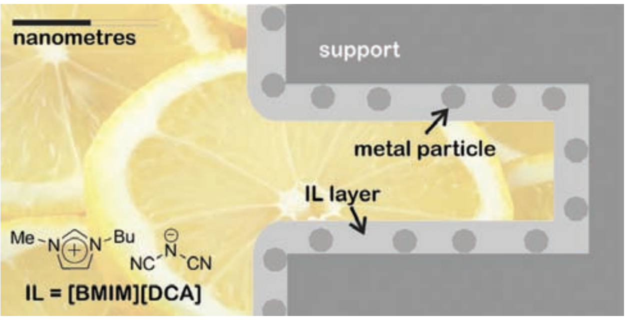
Ionic liquids improve the synthesis of a lemon scented chemical

Sweet smell of success

Scientists from Germany have used ionic liquids to improve the performance of a catalyst that produces citronellal from citral – two compounds that are commonly used as a flavouring and in the perfumery industry, both having a sweet lemon scent.

The hydrogenation of citral is usually performed with a palladium–carbon catalyst. Unfortunately, this reaction does not selectively stop at citronellal, often hydrogenating further to make other products.

Peter Claus and colleagues from the Technical University of Darmstadt have been looking for a catalyst that would produce citronellal selectively. 'This is very important to the chemical industry, where consecutive hydrogenations must very often be prevented,' says Claus.



The ionic liquid (IL) coating improves the hydrogenation catalyst's performance

Ionic liquids are salts in liquid form, and are frequently used as non-volatile solvents and stabilisers in chemical reactions. Claus found that by impregnating an already known Pd/SiO_2 catalyst with an ionic liquid (called butylmethylimidazolium dicyanamide) an almost 100 per cent yield of citronellal is obtained, and very little further hydrogenation occurred.

What's more, by using the ionic liquid as a coating on the catalyst, rather than a bulk solvent, the production cost decreased, and there was no need to separate out the product at the end of the reaction, making the process one step shorter.

Douglas MacFarlane from the ionic liquids group at Monash University, Australia, says this development opens up new areas for catalyst applications. 'This is a fascinating piece of work that shows how effective an ionic liquid layer can be in controlling the selectivity of a conventional solid phase catalyst,' he says.

Rebecca Brodie

Reference

J Arras *et al*, *Chem. Commun.*, 2008, 4058 (DOI: 10.1039/b810291k)

Potent combination of two anticancer molecules synthesised

Natural product hybrid fights cancer

A potent hybrid of two anticancer natural products has been designed and synthesised by UK chemists.

Developing analogues of natural products with improved biological activity is an area of great current interest. Ian Paterson and colleagues at the University of Cambridge have now made a natural product analogue with anticancer activity using a combination of rational design and state-of-the-art synthesis.

Discodermolide is a natural product from marine sponges with high activity against cancer cells. It is currently in clinical trials, but the search is always on for more active analogues. Paterson compared the structure of discodermolide with that of dictyostatin, a more potent but less studied natural product. Using knowledge of the protein binding site involved in the anticancer activity of both molecules, they improved the potency of discodermolide by replacing a part of its structure with a fragment from dictyostatin.

A hybrid of discodermolide (red) and dictyostatin (blue) has been assembled

Both natural products are only available in minute quantities, so the group made their hybrid from scratch. Paterson says that this proved challenging, but that they were able to exploit boron aldol methodology and other synthetic methods to develop 'an efficient and scalable route' to the hybrid.

The hybrid was then tested on four cancer cell lines, and was found to be more potent than discodermolide for all of them. The group also found that deactivating the two hydroxyl groups at the bottom left of the molecule, by tying them up in a ring, resulted in a large drop in activity. This indicates, says Paterson, that one or both of these hydroxyls 'play a key role' in the activity of dictyostatin and discodermolide.

Dennis Curran, from the University of Pittsburgh, US, finds the work very exciting: 'the Paterson group has a flair for analogue design and efficient synthesis, and it looks like they have hit gold with the testing results on this one'. Future work, says Paterson, will involve 'further probing the pharmacophore and anticancer profiles of these fascinating marine natural products and their hybrids'.

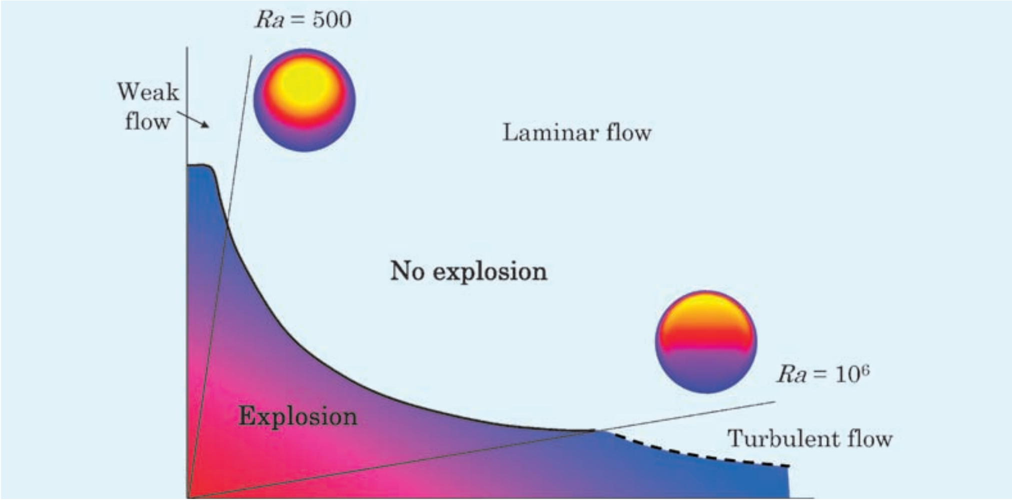
David Barden

Reference

I Paterson, G J Naylor and A E Wright, *Chem. Commun.*, 2008, DOI: 10.1039/b811575c

Is your reaction mixture going to explode? Why not ask a theoretical chemist...

When convection goes without a bang



UK researchers have been investigating how to predict whether a reacting mixture will explode.

Silvana Cardoso and colleagues, at the University of Cambridge, have worked out how to separate the different effects that remove heat from the reaction and hence prevent explosions. These effects are conduction, where the heat flows through material, and convection, where hot material rises away from the reaction site. 'To date', says Cardoso, 'these effects have been analysed in a coupled form. Previously they have been taken into account either in an empirical way, by modifying simpler solutions valid when only heat conduction is present, or in a complex, numerical calculation. Our new treatment allows us to grasp a whole landscape of explosion phenomena which seemed to be unrelated before.'

Cardoso says 'this project aims to develop a more comprehensive theory of explosion, in which the effects of natural convection, as well as those of forced fluid flow, such as by a pump or a stirrer, may be quantified in an explicit manner.' Vitaly Volpert, a mathematician at the University of Lyon, France, identifies the key contribution of the research: 'The interest of the work is that the authors compare the numerical simulations with experimental results, and consider a spherical geometry, which has not been done before.'

Volpert identifies two directions this research could take next, 'If we are talking about fire safety, and this is an important issue, I would say a systematic experimental and theoretical investigation of fuel tanks and so on is needed.' From a theoretical point of view, however, he would like to see a systematic investigation of complex nonlinear dynamics, for example the transition of the behaviour of the combusting system to chaos and chaotic heat explosions.

Colin Batchelor

Theoretical chemists have improved our understanding of why things explode

Reference

T.-Y. Liu *et al*, *Phys. Chem. Chem. Phys.*, 2008, **10**, 5521 (DOI: 10.1039/b808222g)

Researchers step closer to explaining hydrocarbon formation in space

A Titan discovery

The chemistry used to make a rare argon–carbene cation may hold the key to hydrocarbon formation on Saturn's largest moon, claim European researchers.

Detlef Schröder from the Academy of Sciences in Prague, Czech Republic, and co-workers have made a noble-gas compound by colliding argon with dications. Using experimental and theoretical studies they showed that bromomethane (CH_3Br) can be ionised to the molecular dication CH_3Br^{2+} – that can rearrange to the tautomer CH_2BrH^{2+}. The reaction of this dication with argon leads to the argon–carbene cation ($ArCH_2^+$).[1] Schröder also made the corresponding carbene cation for other noble gases, including krypton and xenon.

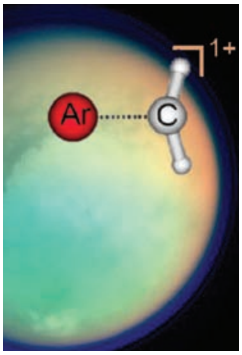
Their work could shed light on the mysteries of the upper part of Titan's atmosphere – the ionosphere – that is known to consist of complex hydrocarbons. Previously scientists have struggled to explain how these are formed.

Stephen Price, from University College London, UK, agrees saying that 'in recent years the bond-forming chemistry of molecular doubly-charged ions has been implicated in environments as varied as the interstellar medium and planetary ionospheres.' And Schröder has shown before that dications are involved in the growth of hydrocarbons on Titan.[2]

Compounds containing noble-gases are rare because they are notoriously difficult to make, with most needing to contain highly electronegative elements – such as fluorine, iodine, oxygen – that are capable of attacking the closed-shell configuration of electrons of the noble gas atoms.

Price adds that, 'the synthesis of argon–carbon bonds using doubly-charged molecular reagents, further extends the range of fields in which the chemistry of gas-phase dications is potentially important.'

Emma Shiells



Hydrocarbon formation in space is poorly understood

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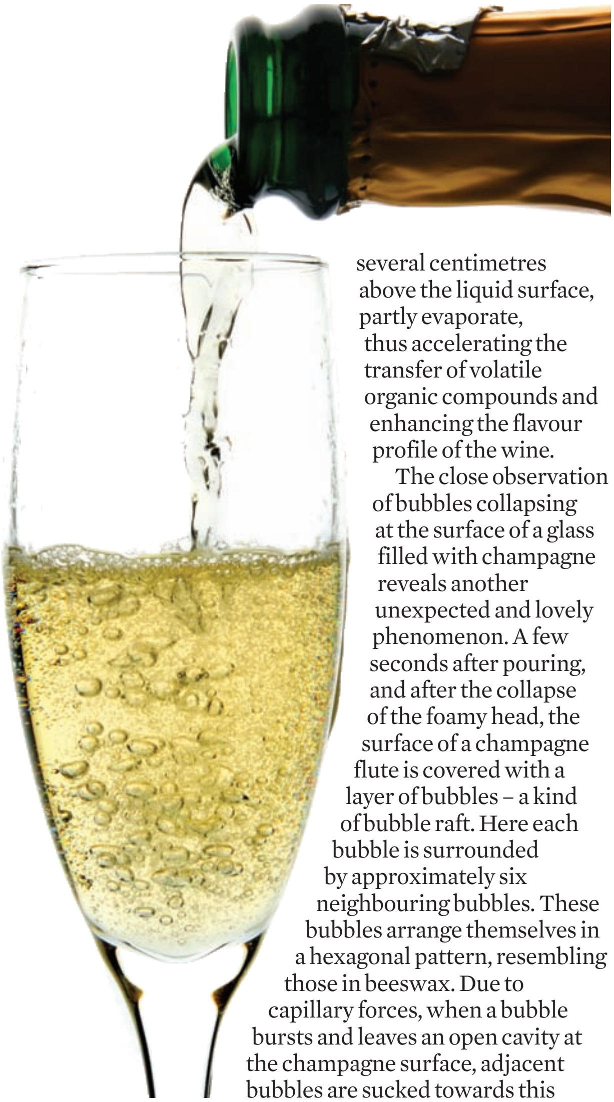
1 D Ascenzi *et al*, *Chem. Commun.*, 2008, 4055 (DOI:10.1039/b811115d)

2 C L. Ricketts *et al*, *Chem. Eur. J.* , 2008, **16**, 4779

Lovely bubbly

Gérard Liger-Belair, University of Reims Champagne-Ardenne, France, celebrates what gives champagne its sparkle



A standard bottle of champagne releases 20 million bubbles

KOLOBO4EK / DREAMSTIME.COM

Since the time of the Benedictine monk Dom Pierre Perignon (1638–1715) champagne is the wine of celebration. With its image inextricably linked to the elegance of its effervescence – the small bubbles it emits.

In champagne and sparkling wines, carbon dioxide molecules form in excess during a unique second fermentation process. And once opened, champagne in a typical 0.75 litre bottle releases approximately five litres of CO_2. This equates to a huge 20 million bubbles formed per bottle.

Bubbles do not just appear as champagne is poured, the dissolved CO_2 molecules must be able to group together and push their way through the liquid molecules. Energetically this is not easy, and close inspection of glasses filled with champagne shows that most of the bubble nucleation (growth) sites are pre-existing gas cavities on the surface of the glass. These gas cavities are trapped inside cellulose fibres on the surface of the glass, that come from the surrounding air or from wiping the glass with a cloth before use.

Recent calculations have linked the final bubbles' size with a combination of their growth rate, the speed with which they ascend and other parameters. The amount of dissolved carbon dioxide content is important: a reduction by a factor of two – which is approximately the factor between champagne and beer – decreases the average bubble size by about 40 %. This is the main reason why, contrary to popular belief, beer bubbles are significantly smaller than those in champagne. The bubble size is also strongly gravity and pressure dependent. On the Moon for example, where the gravity acceleration is only a sixth of that on Earth, bubbles would be about three times larger in volume. And if you could enjoy a glass of champagne on the top of Mount Everest, where the overall pressure is only about 30 per cent of the pressure at the sea level, bubbles would increase by a factor of almost four in volume. This is basically the same phenomenon that is responsible for gas embolism in divers who have breathed high pressure air under water, if they resurface too quickly.

Once formed, bubbles rise toward the liquid surface due to their own buoyancy. While rising, they continue to grow in size by continuously absorbing carbon dioxide molecules dissolved into the champagne. Bubbles therefore continuously accelerate along their way through the champagne. This continuous acceleration can be watched using high speed photographs, where the continuously increasing spacing between the successive bubbles in a given bubble train can be seen. Contrary to popular belief however, champagne bubbles rise at a relatively slow pace (0.5 kilometres per hour), comparable to that of a turtle. That said, when opening a bottle of champagne the release of CO_2 means an uncontrolled cork can reach speeds of 50–60 kilometres per hour!

Without bubbles champagne would be unrecognisable, sparkling wines and beers would be flat. However, the role of effervescence is suspected to go far beyond the sole aesthetical point of view. Bubbles bursting at the liquid surface radiate hundreds of tiny liquid jets which quickly break up into a multitude of tiny droplets every second. Those tiny droplets, ejected up to several centimetres above the liquid surface, partly evaporate, thus accelerating the transfer of volatile organic compounds and enhancing the flavour profile of the wine.

The close observation of bubbles collapsing at the surface of a glass filled with champagne reveals another unexpected and lovely phenomenon. A few seconds after pouring, and after the collapse of the foamy head, the surface of a champagne flute is covered with a layer of bubbles – a kind of bubble raft. Here each bubble is surrounded by approximately six neighbouring bubbles. These bubbles arrange themselves in a hexagonal pattern, resembling those in beeswax. Due to capillary forces, when a bubble bursts and leaves an open cavity at the champagne surface, adjacent bubbles are sucked towards this empty cavity and creating short-lived flower-shaped structures, invisible to the naked eye.

Who would have imagined that a flute of champagne is such a fantastic playground for a chemical physicist in love with microphotography, or for a champagne lover with the time and knowledge to reflect on what is happening right under his nose?

Reference

G Liger-Belair, *Chem. Soc. Rev.*, 2008, DOI: 10.1039/b717798b

Read Gérard Liger-Belair's critical review 'Recent advances in the science of champagne bubbles' in issue 11, 2008 of Chemical Society Reviews.

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Tasting the chemistry

Susan Ebeler, University of California, Davis, US, reveals the science behind the flavour in everyone's favourite tipple

As you sit down to quaff a glass of wine after work, do you ever pause to notice the faint aroma of boxwood, violets or paraffin? Your perception of wine flavour mainly involves four of the five senses – vision, touch, taste and smell. And it is our nose that gives the greatest contribution to the flavour by detecting the aroma of hundreds of volatile chemical compounds in the wine. The compounds responsible for the smells above are – at low concentrations – typically present in popular grape varieties such as Sauvignon blanc, Pinot noir and Riesling.

As you reach the end of the bottle do you ever start to ponder about the people who make your wine? It may surprise you to learn that science – including analytical chemistry, sensory science, genetics and molecular biology – plays a large part in providing much of the information needed by wineries to make their wine as appealing as possible to our senses. This includes knowledge of the chemical compounds that contribute to wine flavour, how this flavour is formed during grape growth and the winemaking process, how humans perceive flavour compounds and how human genetics can influence individual perception of smells.

Over 1000 different aroma compounds in grapes and wines have now been identified using various analytical tools. Gas chromatography, one of the most powerful tools for separating complex mixtures into individual components, has been widely used for this purpose since the 1950s. However, sensitivity to aromas varies significantly from person to person, so not all volatile compounds that are identified using analytical tools will actually contribute to what you smell. Conversely, sometimes our sensitivity far exceeds that of the analytical chemist's tools.

JUPITER IMAGES

The aroma of the compound that contributes to bell pepper aroma in many Sauvignon blanc and Cabernet Sauvignon wines for example can be sensed by humans at concentrations as low as 2 ng per litre – that's equivalent to two drops mixed into 20 Olympic size swimming pools – far below what any analytical technique can currently sense without special sampling or extraction techniques. New methods for preparing and extracting samples are now allowing scientists to push the limits of analytical detection without requiring litres and litres of sample. Additionally by combining gas chromatography with the human sense of smell, in a technique called gas chromatography-olfactometry, scientists can now isolate the 15–20 chemical compounds that contribute the most to wine aroma from the hundreds or thousands of compounds identified in a specific wine.

Wine aroma is further complicated by interactions between volatile aroma, and non-aroma, compounds. The interactions mean that two aroma compounds may smell differently when mixed together. Additionally a strong fruity aroma can also mask a weaker vegetable aroma in a wine.

We have scientists to thank for the delicious taste of both fruity red and crisp white wine

Using a combination of sensory and analytical tools, and an improved understanding of the genetics, physiology and neurobiology of how humans perceive smells, scientists are ever improving our knowledge of the factors that contribute to overall wine aroma perception.

Molecular biologists are also studying how plant and yeast genes impact aroma formation in the grape and during fermentation, improving our understanding of the biochemical processes involved in flavour formation.

Armed with this knowledge, viticulturists and winemakers can study how vineyard practices – such as soil conditions, irrigation and fertilisation – and winemaking processes – such as choice of yeast strain, fermentation temperature, yeast nutrients, oxygen exposure – impact the chemical composition and sensory properties of their wine. All this information allows winemakers to identify grape varieties, yeast strains, and fermentation conditions that will yield desired flavour properties for specific wine styles and consumer preferences.

I suspect you didn't realise the chemistry in a glass of wine is quite so complex. So, the next time you enjoy a glass of fine wine take time to toast the chemists, plant scientists, viticulturists and winemakers who've used the latest scientific tools to ensure that it tastes and smells the way you know and love.

Read Pavla Polášková, Julian Herszage and Susan Ebeler's critical review 'Wine flavor: chemistry in a glass' in issue 11, 2008 of Chemical Society Reviews

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Reference

P Polášková *et al*, *Chem. Soc. Rev.*, 2008, DOI: 10.1039/b714455p

Essential elements

Engineering success

CrystEngComm celebrated its tenth year of publication in style on 28 August with a lunch reception held at the XXI Congress and General Assembly of the International Union of Crystallography in Osaka, Japan. As part of the celebrations, the journal also awarded five poster prizes at the meeting.

Since its launch in 1999, *CrystEngComm* has gone from strength to strength, growing in size by more than a factor of ten. The journal now boasts the fastest publication times and highest immediacy index for a crystal engineering journal, plus an impressive impact factor of 3.47. In his welcome speech, *CrystEngComm* editor Jamie Humphrey outlined the successes of the past decade and extended his thanks: 'This success has been possible only through the support that you and other members of the crystal engineering community have given the journal – your support as authors, referees, readers and in some cases editorial and advisory board members.'

Regular *CrystEngComm* author Pierangelo Metrangolo of Milan, Italy, who attended the lunch reception, cites the journal as one of his favourites for publication of his research. 'In particular,' he says, 'I appreciate the speed at which papers are processed and the very kind co-operation of the editorial staff. What else to say: Happy Birthday *CrystEngComm*..., and keep up the good work!'

A decade since launch and the future for *CrystEngComm* has never looked so bright. Celebrations will continue later this year with an anniversary theme issue, including articles by editorial and advisory board members, and the journal is also heavily involved in the organisation of a crystal engineering symposium as part of the IUPAC Congress next year in Glasgow.

Visit www.crystengcomm.org for updates on these and other exciting events.

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Or paste the following URL into your browser: www.facebook.com/pages/Energy-Environmental-Science/24375018213.

See you there!

A warm reception in Philadelphia

The atmosphere inside the Philadelphia Marriott mirrored the sunny blue sky outside as guests gathered at the RSC Reception. Held on 17 August, it coincided with the 236th American Chemical Society National Meeting and Exposition taking place at the Pennsylvania Convention Center.

Left to right: Jonathan Sessler (U Texas at Austin), Kate Sear (deputy editor ChemComm, RSC), Kevin Burgess (Texas A&M), Peter Wipf (Pittsburgh)

Around 200 people listened to RSC president Dave Garner as he welcomed guests, including Nobel prize winner Bob Grubbs from Caltech, a variety of eminent and emerging researchers, plus university librarians and local RSC members. The incoming president of the ACS, Tom Lane, was also there with a number of his society colleagues, indicating the continuing warm friendship between the two chemical societies.

Guests enjoyed refreshments while catching up with friends old and new, and RSC staff were on hand to describe the latest RSC initiatives, including the hot topics of *Energy & Environmental Science*, *Integrative Biology* and *Metallomics*, the three newest RSC journals.

At the end of a genial evening, everyone was looking forward to meeting again – so see you all in Salt Lake City in spring 2009!

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