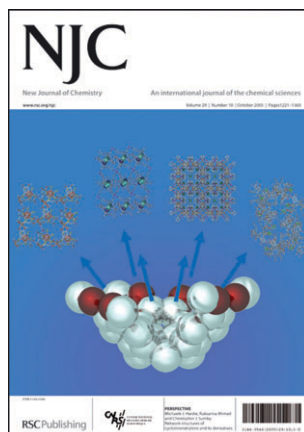


## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 29(10) 1221-1360 (2005)

## In this issue...

Stéphane Daniele describes the cooperative combination of two catalytic sites in a mesoporous nanocrystalline  $\text{TiO}_2$ -iron tetrasulfophthalocyanine material to provide good catalytic oxidation properties. See p. 1245



## Cover

See Michael J. Hardie *et al.*, page 1231. The cover shows the molecular host cyclotrimeratrylene incorporated into 2-D and 3-D network structures through hydrogen bonding and/or coordination interactions. Utilising minimal synthetic organic chemistry pyridyl ligand groups can be appended to the host framework providing new derivatives capable of forming robust transition metal based coordination networks.

Image reproduced by permission of Michael J. Hardie, Ruksanna Ahmad and Christopher J. Sumby, *New J. Chem.*, 2005, 29, 1231.

## CHEMICAL SCIENCE

C73

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

# Chemical Science

October 2005/Volume 2/Issue 10

[www.rsc.org/chemicalscience](http://www.rsc.org/chemicalscience)

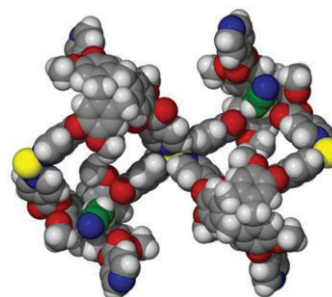
## PERSPECTIVE

1231

## Network structures of cyclotrimeratrylene and its derivatives

Michael J. Hardie,\* Ruksanna Ahmad and Christopher J. Sumby

The host molecule cyclotrimeratrylene, and pyridyl-functionalised derivatives, can be incorporated into hydrogen bonded networks and/or coordination networks. The resultant network structures show a range of chain, 2-D and 3-D structures, with hexagonal  $6^3$  nets predominating.





## EDITORIAL STAFF

**Managing editor (RSC)**

Mike Corkill

**Managing editor (CNRS)**

Denise Parent

**Assistant managing editor**

G  rard Calleja (CNRS)

**Publishing assistant**

Jackie Cockrill (RSC)

**Team leader, serials production**

Helen Saxton (RSC)

**Technical editors**

Caroline Moore (RSC), Celia Clarke (RSC), Ken Wilkinson (RSC)

**Administration coordinator**

Sonya Spring (RSC)

**Editorial secretaries**

Lynne Braybrook (RSC), Rebecca Gotobed (RSC), Florence Lepage (CNRS), Julie Thompson (RSC)

**Publisher**

Adrian Kybett (RSC)

New Journal of Chemistry (Print: ISSN 1144-0546; electronic: ISSN 1369-9261) is published 12 times a year by the Centre National de la Recherche Scientifique (CNRS), 3 rue Michel-Ange, 75794 Paris cedex 16, France, and the Royal Society of Chemistry (RSC), Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to RSC Distribution Services, c/o Portland Customer Services, Commerce Way, Colchester, Essex, UK CO2 8HP, UK. Tel +44 (0) 1206 226050; E-mail sales@rscdistribution.org

2005 Annual (print + electronic) subscription price:   650; US\$1075. 2005 Annual (electronic) subscription price:   585; US\$965. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any RSC journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at [www.rsc.org/ip](http://www.rsc.org/ip). Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank. Periodicals postage paid at Rahway, NJ, USA and at additional mailing offices. Airfreight and mailing in the USA by Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001, USA.

US Postmaster: send address changes to New Journal of Chemistry, c/o Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001. All despatches outside the UK by Consolidated Airfreight.

PRINTED IN THE UK

**Advertisement sales:** Tel +44 (0) 1223 432243; Fax +44 (0) 1223 426017; E-mail [advertising@rsc.org](mailto:advertising@rsc.org)

NJC

New Journal of Chemistry

An international journal for the chemical sciences

[www.rsc.org/njc](http://www.rsc.org/njc)

The New Journal of Chemistry is a broad-based primary journal encompassing all branches of the chemical sciences. Published monthly, it contains full research articles, letters, opinions and perspectives.

## EDITORIAL BOARD

**Editor-in-chief**

Jean-Pierre Majoral, Toulouse, France

**Consulting editor**

Odile Eisenstein, Montpellier, France

**Board members**

Laurent Bonnevot, Lyon, France  
John A Gladysz, Erlangen, Germany  
George Gokel, St Louis, MO, USA  
Luca Prodi, Bologna, Italy  
Paul Raithby, Bath, UK  
David Reinhoudt, Enschede, The Netherlands

Alan Rowan, Nijmegen, The Netherlands  
Michael Scott, Gainesville, FL, USA  
Jonathan W Steed, Durham, UK  
Michael Veith, Saarbr  cken, Germany  
Vivian Yam, Hong Kong, PR China

**Associate editors**

Manuscripts should be directed to the appropriate Editor detailed below.

**Supramolecular chemistry and crystal engineering**

Dr Jonathan W Steed  
Department of Chemistry  
University Science Laboratories  
University of Durham  
South Road  
Durham  
UK DH1 3LE  
Fax (+44) (0) 191 384 4737  
Tel (+44) (0) 191 384 2085  
E-mail [jon.steed@dur.ac.uk](mailto:jon.steed@dur.ac.uk)

**Organic & bioorganic**

Professor George Gokel  
Departments of Chemistry and  
Molecular Biology & Pharmacology  
Washington University Medical  
School  
Campus Box 8103  
660 S. Euclid Ave.  
St Louis, MO 63110, USA  
Fax (+1) 314 362 9298  
Tel (+1) 314 362 9297  
E-mail [ggokel@molecool.wustl.edu](mailto:ggokel@molecool.wustl.edu)

Alternatively, any author may submit direct to the  
**Montpellier Editorial Office**  
Dr Denise Parent  
New Journal of Chemistry  
Universit   Montpellier II  
Place Eug  ne Bataillon  
C.C. 014  
34095 Montpellier cedex 5  
France  
Fax (+33) (0) 4 67 14 48 79  
Tel (+33) (0) 4 67 14 48 78  
E-mail [njc@univ-montp2.fr](mailto:njc@univ-montp2.fr)

## INTERNATIONAL ADVISORY EDITORIAL BOARD

Markus Antonietti, MPI, Potsdam, Germany  
Didier Astruc, Talence, France  
Jerry Atwood, Columbia, MO, USA  
Pierre Braunstein, Strasbourg, France  
Kenneth Caulton, Bloomington, IN, USA  
Robert Crabtree, New Haven, CT, USA  
Pierre Dixneuf, Rennes, France

Fran  ois Fajula, Montpellier, France  
Andrew B Holmes, Melbourne, Australia  
Reinhard W Hoffmann, Marburg, Germany  
Miguel Julve, Valencia, Spain  
Peter Junk, Monash, Australia  
Henryk Koslowski, Wroclaw, Poland  
Bernard Meunier, Toulouse, France

Jan Reedijk, Leiden, The Netherlands  
Kari Rissanen, Jyv  skyl  , Finland  
Cl  ment Sanchez, Paris, France  
Jeremy K M Sanders, Cambridge, UK  
Philippe Sautet, Lyon, France  
Jean-Pierre Sauvage, Strasbourg, France  
Ulrich Schubert, Vienna, Austria  
Hideki Sugihara, Tsukuba, Japan

## INFORMATION FOR AUTHORS

Full details of how to submit material for publication in the New Journal of Chemistry are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be sent via ReSource: <http://www.rsc.org/resource>. Authors may reproduce/republish portions of their published contribution without seeking permission from the CNRS and the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation) – Reproduced by permission of the CNRS and the RSC.

  The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2005. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulations 2003, this publication may

only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of The Royal Society of Chemistry or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions.

  The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

Royal Society of Chemistry: Registered Charity No. 207890



## LETTERS

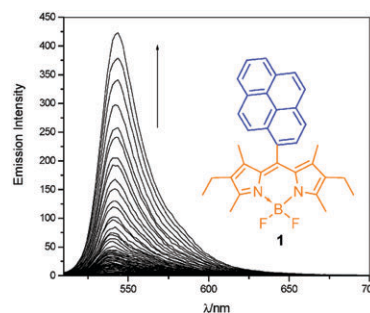
1241



### Engineering of an electronically decoupled difluoroindacene-pyrene dyad possessing high affinity for DNA

James P. Rostron, Gilles Ulrich, Pascal Retailleau, Anthony Harriman\* and Raymond Ziessel\*

Progressive addition of compound **1** to a DNA solution resulted in a quenching of the luminescence due to aggregation of the molecules, followed by the increasing of luminescence of the free dye after filling of the major groove of the DNA strands.

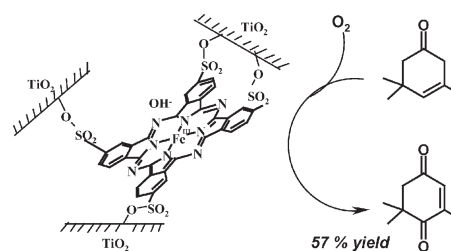


1245

### Combination of two catalytic sites in a novel nanocrystalline TiO<sub>2</sub>-iron tetrasulfophthalocyanine material provides better catalytic properties

Mirvat Beyrhouty, Alexander B. Sorokin,\* Stéphane Daniele\* and Liliane G. Hubert-Pfalzgraf

Fixation of iron phthalocyanine on to TiO<sub>2</sub> affords an improved catalyst for aerobic heterogeneous oxidation of β-isophorone to ketoisophorone, a valuable intermediate for fragrance chemistry.



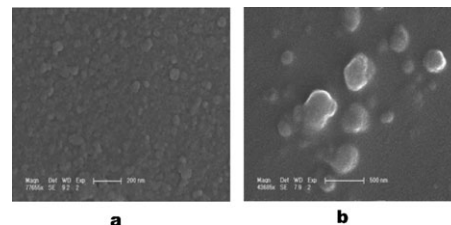
## PAPERS

1249

### Nucleation and growth of polyoxometalate nanoparticles in polyelectrolyte multilayer films

Yang Lan, Enbo Wang,\* Yonghai Song, Zhenhui Kang, Lin Xu, Zhuang Li and Meiye Li

The *in situ* controllable formation of polyoxometalate nanoparticles, of varying size and morphology, in poly(diallyldimethylammonium chloride) and poly(styrenesulfonate) sodium salt composite films has been achieved by using layer-by-layer electrostatic assembly.



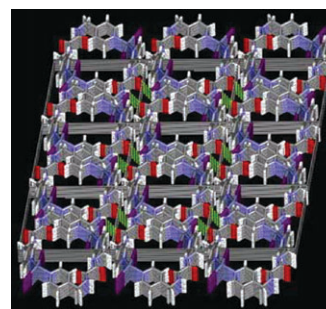
1254



### Anion-directed assembly of supramolecular zinc(II) halides with *N,N'*-bis-4-methyl-pyridyl oxalamide

Biing-Chiau Tzeng,\* Bo-So Chen, Shih-Yang Lee, Wei-Hsin Liu, Gene-Hsiang Lee and Shie-Ming Peng

A molecular rectangle with a rectangular cavity of *ca.* 6.4 × 11.0 Å<sup>2</sup> is formed and further stacked to give one-dimensional rectangular channels in the solid state. This is reminiscent of the interesting nanotube frameworks of cyclic peptides.





1258



### A study of the effects of subunit pre-orientation for diarylpyrrole esters; design of new aryl-heteroaryl fluorescent sensors

John Killoran, John F. Gallagher, Paul V. Murphy and Donal F. O'Shea\*

Elucidation of the design principles for aryl-heteroaryl fluorescent sensors based upon the pre-orientation of the sensor subunits.

1266



### Hydrogen-bonded chains of $\alpha,\omega$ -diaminoalkane and $\alpha,\omega$ -dihydroxyalkane guest molecules lead to disrupted tunnel structures in urea inclusion compounds

Sang-Ok Lee, Benson M. Kariuki and Kenneth D. M. Harris\*

Structural features of urea inclusion compounds containing 1 : 1 mixtures of  $\alpha,\omega$ -diaminoalkane and  $\alpha,\omega$ -dihydroxyalkane guest molecules provide interesting contrasts to those of conventional urea inclusion compounds.

1272

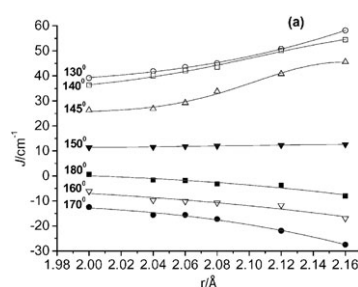


### Distance-independent photoinduced energy transfer over 1.1 to 2.3 nm in ruthenium trisbipyridine–fullerene assemblies

Frédérique Chaignon, Javier Torroba, Errol Blart, Magnus Borgström, Leif Hammarström\* and Fabrice Odobel\*

Light excitation of ruthenium trisbipyridine complex in the dyads results in a quantitative photoinduced energy transfer to form the fullerene triplet excited state.

1285

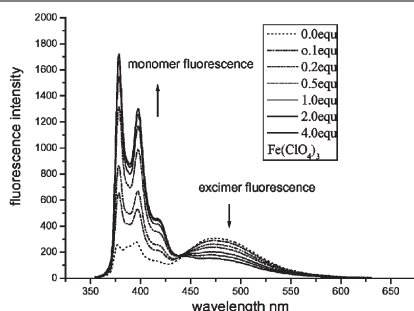


### Exchange coupling behavior of cyano-bridged binuclear Fe(III)–Ni(II) complexes: a density functional theory combined with broken-symmetry approach

Yi-Quan Zhang,\* Cheng-Lin Luo and Zhi Yu

Magnetic coupling constant  $J$  as a function of the  $r$  distance ranging from 2.0 Å to 2.16 Å for model 1 when the angle is 130°, 140°, 145°, 150°, 160°, 170° and 180°, respectively.

1291



### Novel redox-fluorescence switch based on a triad containing tetrathiafulvalene and pyrene units with tunable monomer and excimer emissions

Xunwen Xiao, Wei Xu,\* Deqing Zhang, Hai Xu, Lei Liu and Daoben Zhu\*

A new fluorescence switch with tunable pyrene monomer and excimer emissions was achieved by the collective result of the tunable photoinduced electron transfer and resonance energy transfer processes.

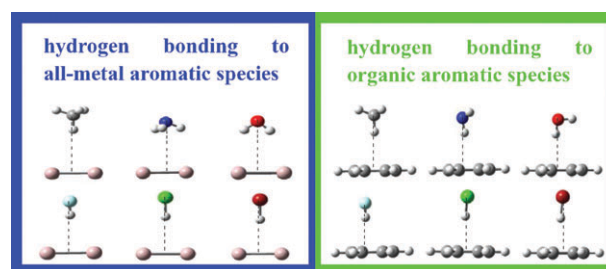


1295

### Exploring a new kind of aromatic hydrogen bond: hydrogen bonding to all-metal aromatic species

Xingbang Hu, Haoran Li,\* Wanchun Liang and Shijun Han

Based on the recent advance of the aromaticity concept into all-metal species, we put forward a new kind of hydrogen bond: hydrogen bonding to all-metal aromatic species.

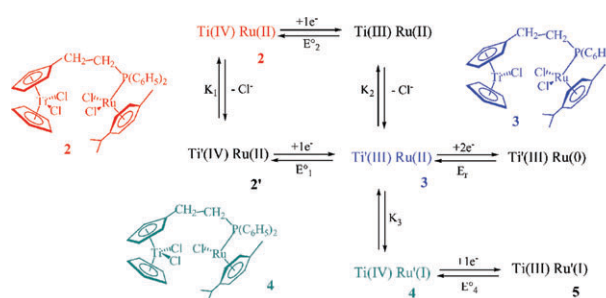


1302

### Evidence of intramolecular electron transfer between two metallic atoms in a bimetallic complex by electrochemical methods

Hélène Cattey,\* Alain Vallat, Pierre Le Gendre, David Evrard, Claude Moïse and Yves Mugnier

The electrochemical activity of the complex **2** has revealed an unexpected intramolecular electron transfer between the two metallic atoms *via* a chloride atom transfer (complexes **3** to **4**).

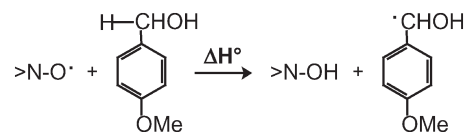


1308

### New mediators for the enzyme laccase: mechanistic features and selectivity in the oxidation of non-phenolic substrates

Paola Astolfi, Paolo Brandi, Carlo Galli,\* Patrizia Gentili,\* Maria Francesca Gerini, Lucedio Greci and Osvaldo Lanzalunga

New mediators of laccase are evaluated, their mechanism of oxidation with benzyl alcohols discussed, and the dissociation energy of the O–H bond of 1-hydroxybenzotriazole calculated.

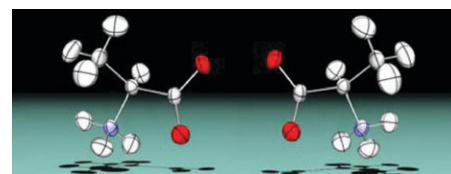


1318

### Neutron diffraction investigations of L- and D-alanine at different temperatures: the search for structural evidence for parity violation

Chick C. Wilson,\* Dean Myles, Minakshi Ghosh, Louise N. Johnson and Wenging Wang

Detailed neutron diffraction studies of L- and D-alanine yield no structural evidence for the proposed phase transition in this amino acid, thus offering no structural basis for the observable effect of parity violation of the electroweak force in these phase transitions.

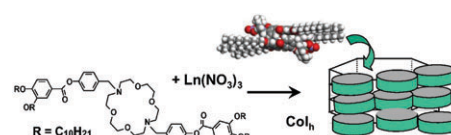


1323

### Lanthanide luminescent mesomorphic complexes with macrocycles derived from diaza-18-crown-6

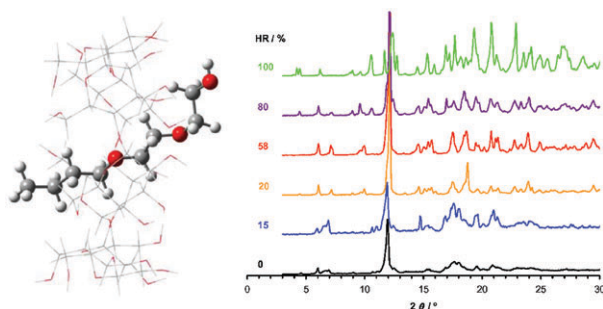
Stéphane Suárez, Olimpia Mamula, Rosario Scopelliti, Bertrand Donnio, Daniel Guillon, Emmanuel Terazzi, Claude Piguet and Jean-Claude G. Bünzli\*

A tetracatenar ligand derived from the diaza-18-crown-6 framework reacts with lanthanide nitrates to yield luminescent hexagonal columnar liquid crystalline phases (Col<sub>h</sub>), extending over a temperature range larger than 100 °C.





1335



### Solid-state inclusion compounds of small amphiphilic molecules ( $C_nE_m$ ) in $\beta$ -cyclodextrin: a study at defined relative humidities

Luís Cunha-Silva\* and José J. C. Teixeira-Dias

Solid-inclusion compounds of  $C_4E_1$ ,  $C_4E_2$  and  $C_6E_2$  in  $\beta$ CD were prepared and studied by PXRD, TGA, FT-Raman and  $^{13}\text{C}$  CP MAS NMR spectroscopy, at ambient humidity and several defined relative humidities.

1342

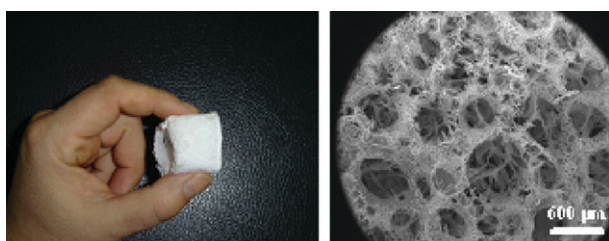


### Nanosized metallic particles embedded in silica and carbon aerogels as catalysts in the Mizoroki–Heck coupling reaction

Sandra Martínez, Adelina Vallribera,\* Cosmin L. Cotet, Mihaela Popovici, Laura Martín, Anna Roig,\* Marcial Moreno-Mañas and Elies Molins

Various aerogels containing Ni and Pd nanoparticles have been prepared by sol-gel processes. The organic and carbon aerogels doped with Pd are good catalysts for the Mizoroki–Heck reaction.

1346

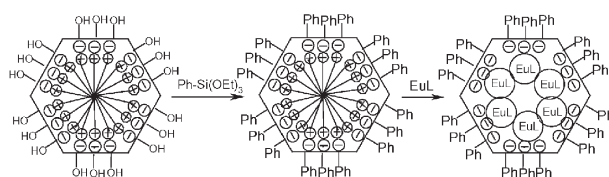


### Shaping zirconium phosphate $\alpha\text{-Zr}(\text{HPO}_4)_2 \cdot \text{H}_2\text{O}$ : from exfoliation to first $\alpha\text{-ZrP}$ 3D open-cell macrocellular foams

Florent Carn, Alain Derré, Wilfrid Neri, Odile Babot, Hervé Deleuze and Rénal Backov\*

Using a two-step exfoliation–foaming process the first  $\alpha\text{-ZrP}$  3D open-cell macrocellular foams have been obtained with strong design both over cell morphologies and shapes.

1351



### Incorporation of luminescent lanthanide complex inside the channels of organically modified mesoporous silica *via* template-ion exchange method

Xianmin Guo, Lianshe Fu,\* Hongjie Zhang,\* L. D. Carlos, Chunyun Peng, Junfang Guo, Jiangbo Yu, Ruiping Deng and Lining Sun

Lanthanide complex was incorporated into the channels of MCM-41 with its external surface modified by phenyltriethoxysilane *via* template-ion exchange method.



## AUTHOR INDEX

- Ahmad, Ruksana, 1231  
 Astolfi, Paola, 1308  
 Babot, Odile, 1346  
 Backov, Rénal, 1346  
 Beyrhouty, Mirvat, 1245  
 Blart, Errol, 1272  
 Borgström, Magnus, 1272  
 Brandi, Paolo, 1308  
 Bünzli, Jean-Claude G., 1323  
 Carlos, L. D., 1351  
 Carn, Florent, 1346  
 Cattet, Hélène, 1302  
 Chaignon, Frédérique, 1272  
 Chen, Bo-So, 1254  
 Cotet, Cosmin L., 1342  
 Cunha-Silva, Luís, 1335  
 Daniele, Stéphane, 1245  
 Deleuze, Hervé, 1346  
 Deng, Ruiping, 1351  
 Derré, Alain, 1346  
 Donnio, Bertrand, 1323  
 Evrard, David, 1302  
 Fu, Lianshe, 1351  
 Gallagher, John F., 1258  
 Galli, Carlo, 1308  
 Gentili, Patrizia, 1308  
 Gerini, Maria Francesca, 1308  
 Ghosh, Minakshi, 1318  
 Greci, Lucedio, 1308  
 Guillon, Daniel, 1323  
 Guo, Junfang, 1351  
 Guo, Xianmin, 1351  
 Hammarström, Leif, 1272  
 Han, Shijun, 1295  
 Hardie, Michael J., 1231  
 Harriman, Anthony, 1241  
 Harris, Kenneth D. M., 1266  
 Hu, Xingbang, 1295  
 Hubert-Pfalzgraf, Liliane G., 1245  
 Johnson, Louise N., 1318  
 Kang, Zhenhui, 1249  
 Kariuki, Benson M., 1266  
 Killoran, John, 1258  
 Lan, Yang, 1249  
 Lanzalunga, Osvaldo, 1308  
 Le Gendre, Pierre, 1302  
 Lee, Gene-Hsiang, 1254  
 Lee, Sang-Ok, 1266  
 Lee, Shih-Yang, 1254  
 Li, Haoran, 1295  
 Li, Meiyue, 1249  
 Li, Zhuang, 1249  
 Liang, Wanchun, 1295  
 Liu, Lei, 1291  
 Liu, Wei-Hsin, 1254  
 Luo, Cheng-Lin, 1285  
 Mamula, Olimpia, 1323  
 Martín, Laura, 1342  
 Martínez, Sandra, 1342  
 Moise, Claude, 1302  
 Molins, Elies, 1342  
 Moreno-Mañas, Marcial, 1342  
 Mugnier, Yves, 1302  
 Murphy, Paul V., 1258  
 Myles, Dean, 1318  
 Neri, Wilfrid, 1346  
 Odobel, Fabrice, 1272  
 O'Shea, Donal F., 1258  
 Peng, Chunyun, 1351  
 Peng, Shie-Ming, 1254  
 Piguet, Claude, 1323  
 Popovici, Mihaela, 1342  
 Retailleau, Pascal, 1241  
 Roig, Anna, 1342  
 Rostron, James P., 1241  
 Scopelliti, Rosario, 1323  
 Song, Yonghai, 1249  
 Sorokin, Alexander B., 1245  
 Suárez, Stéphane, 1323  
 Sumby, Christopher J., 1231  
 Sun, Lining, 1351  
 Teixeira-Dias, José J. C., 1335  
 Terazzi, Emmanuel, 1323  
 Torroba, Javier, 1272  
 Tzeng, Bing-Chiau, 1254  
 Ulrich, Gilles, 1241  
 Vallat, Alain, 1302  
 Vallribera, Adelina, 1342  
 Wang, Enbo, 1249  
 Wang, Wenging, 1318  
 Wilson, Chick C., 1318  
 Xiao, Xunwen, 1291  
 Xu, Hai, 1291  
 Xu, Lin, 1249  
 Xu, Wei, 1291  
 Yu, Jiangbo, 1351  
 Yu, Zhi, 1285  
 Zhang, Deqing, 1291  
 Zhang, Hongjie, 1351  
 Zhang, Yi-Quan, 1285  
 Zhu, Daoben, 1291  
 Ziessel, Raymond, 1241

## FREE E-MAIL ALERTS

Contents lists in advance of publication are available on the web via [www.rsc.org/njc](http://www.rsc.org/njc) – or take advantage of our free e-mail alerting service ([www.rsc.org/ej\\_alert](http://www.rsc.org/ej_alert)) to receive notification each time a new list becomes available.

\* Indicates the author for correspondence: see article for details.



Electronic supplementary information (ESI) is available via the online article (see <http://www.rsc.org/esi> for general information about ESI).

## ADVANCE ARTICLES AND ELECTRONIC JOURNAL

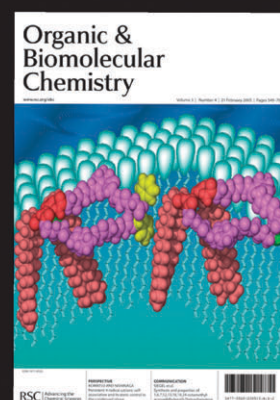
Free site-wide access to Advance Articles and the electronic form of this journal is provided with a full-rate institutional subscription. See [www.rsc.org/ejs](http://www.rsc.org/ejs) for more information.

# Organic & Biomolecular Chemistry

A major peer-reviewed international, high quality journal covering the full breadth of synthetic, physical and biomolecular organic chemistry.

Publish your review, article, or communication in OBC and benefit from:

- The fastest times to publication (80 days for full papers, 40 days for communications)
- High visibility (OBC is indexed in MEDLINE)
- Free colour (where scientifically justified)
- Electronic submission and manuscript tracking via ReSource ([www.rsc.org/ReSource](http://www.rsc.org/ReSource))
- A first class professional service
- No page charges



**Submit today!**

RSC Publishing

[www.rsc.org/obc](http://www.rsc.org/obc)



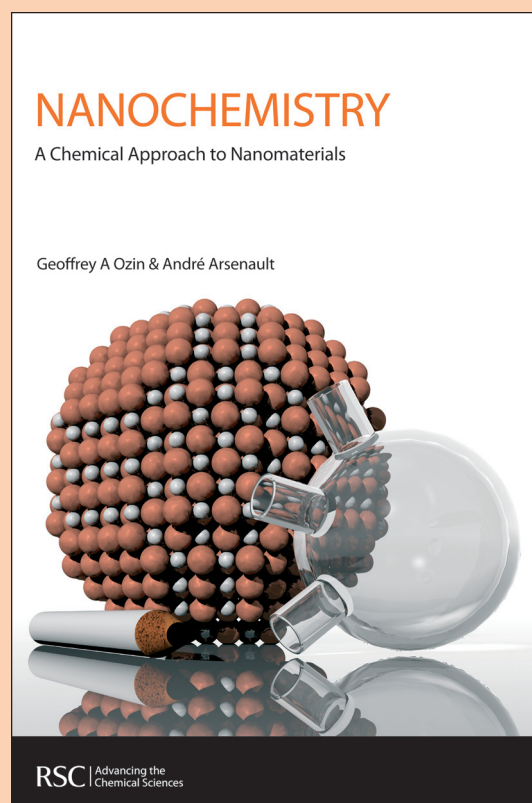
# The first textbook in the field

# NANOCHEMISTRY

## A Chemical Approach to Nanomaterials

By Geoffrey A Ozin and André C Arsenault

- Interdisciplinary and comprehensive
- Presents a basic chemical strategy for making nanomaterials
- Describes some of the principles of materials self-assembly over 'all' scales
- Demonstrates nanometre and micrometre scale building blocks
- Suggests new ways to tackle research problems
- Includes speculations on how to think about assembling the future of nanotechnology



*Nanochemistry: A Chemical Approach to Nanomaterials* is well illustrated with graphical representations of the structure and form of nanomaterials. It contains many pedagogical features and will appeal to graduate and advanced undergraduate students.

Hardcover | 0 85404 664 X | 2005 | 594 pages | £39.95 | RSC member price £25.75

RSC Publishing

[www.rsc.org/books/nanochemistry](http://www.rsc.org/books/nanochemistry)