

CrystEngComm

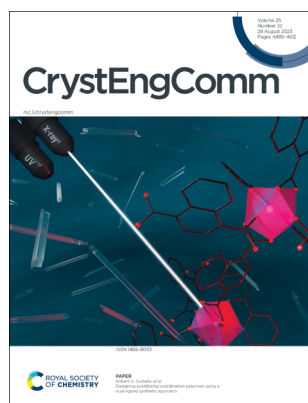
A journal at the forefront of the design and understanding of solid-state and crystalline materials

rsc.li/crystengcomm

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

IN THIS ISSUE

ISSN 1466-8033 CODEN CRECF4 25(32) 4489-4612 (2023)



Cover

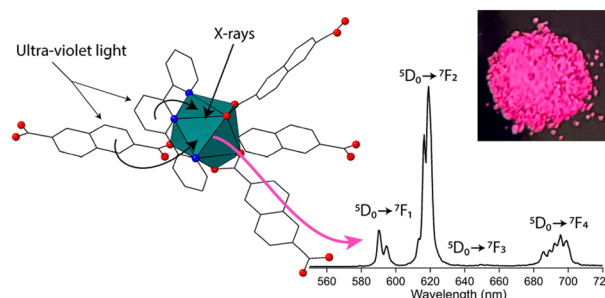
See Robert G. Surbella et al., pp. 4496–4502.
Image reproduced by permission of Battelle Memorial Institute from *CrystEngComm*, 2023, 25, 4496.

PAPERS

4496

Designing scintillating coordination polymers using a dual-ligand synthetic approach

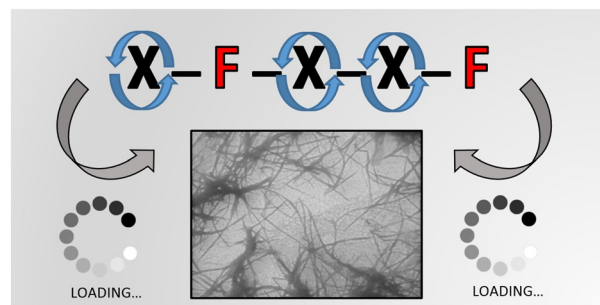
Ana Arteaga, Alice Lulich, May Nyman and Robert G. Surbella III*



4503

Computation meets experiment: identification of highly efficient fibrillating peptides

Lorenzo Sori, Andrea Pizzi,* Greta Bergamaschi, Alessandro Gori, Alfonso Gautieri, Nicola Demitri, Monica Soncini and Pierangelo Metrangolo*



Editorial Staff

Executive Editor

Sally Howells

Deputy Editor

Mike Andrews

Development Editors

Samantha Apps, Michelle Canning

Editorial Production Manager

Susannah Davies

Publishing Editors

Debora Giovannelli, Helen Lunn, Samuel Oldknow, Kate Tustain

Editorial Assistant

Daphne Houston

Publishing Assistant

Huw Hedges

Publisher

Jeanne Andres

For queries about submitted articles please contact
Susannah Davies, Editorial Production Manager in the first
instance. E-mail crystengcomm@rsc.org

For pre-submission queries please contact
Sally Howells, Editor.

Email crystengcomm-rsc@rsc.org

CrystEngComm (electronic: ISSN 1466-8033) is published
48 times a year by the Royal Society of Chemistry,
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 the Royal Society of Chemistry
Order Department, Royal Society of Chemistry,
Thomas Graham House, Science Park, Milton Road,
Cambridge, CB4 0WF, UK

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

2022 Annual (electronic) subscription price: £1268; US\$1883.
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 Royal Society of
Chemistry 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

Customers should make payments by cheque in sterling
payable on a UK clearing bank or in US dollars payable
on a US clearing bank.

Whilst this material has been produced with all due care, the
Royal Society of Chemistry cannot be held responsible or liable
for its accuracy and completeness, nor for any consequences
arising from any errors or the use of the information contained
in this publication. The publication of advertisements does
not constitute any endorsement by the Royal Society of
Chemistry or Authors of any products advertised. The views
and opinions advanced by contributors do not necessarily
reflect those of the Royal Society of Chemistry which shall not
be liable for any resulting loss or damage arising as a result of
reliance upon this material. The Royal Society of Chemistry is
a charity, registered in England and Wales, Number 207890,
and a company incorporated in England by Royal Charter
(Registered No. RC000524), registered office:
Burlington House, Piccadilly, London W1J 0BA, UK,
Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017;

E-mail advertising@rsc.org

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

CrystEngComm

A journal at the forefront of the design and understanding of solid-state and
crystalline materials

rsc.li/crystengcomm

CrystEngComm is the forum for the design and understanding of crystalline materials.
We welcome studies on the investigation of molecular behaviour within crystals, control
of nucleation and crystal growth, engineering of crystal structures, and construction of
crystalline materials with tuneable properties and functions.

Editorial Board

Chair

Pierangelo Metrangolo, Politecnico di Milano,
Italy

Associate Editors

Susan Bourne, University of Cape Town,
South Africa
Christian Doonan, The University of Adelaide,
Australia
Kwangyeol Lee, Korea University, South Korea
C. Malla Reddy, IISER Kolkata, India
Dongfeng Xue, Multiscale Crystal Materials
Research Center of Shenzhen Institute of
Advanced Technology of CAS, China

Members

Elena Boldyreva, Novosibirsk State University,
Russia
Aurora Cruz-Cabeza, Durham University, UK
Omar Farha, Northwestern University, USA
Tong-Bu Lu, Tianjin University of Technology,
China
Susan M. Reutzel-Edens, The Cambridge
Crystallographic Data Centre, UK

Advisory Board

Christer Aakeroy, Kansas State University, USA
Srinivasulu Aitipamula, Institute of Chemical
and Engineering Sciences, Singapore
Alessia Bacchi, University of Parma, Italy
Rahul Banerjee, IISER Kolkata, India
Leonard Barbour, University of
Stellenbosch, South Africa
Andrew Bond, University of Cambridge, UK
Paola Ceroni, University of Bologna, Italy
Deepak Chopra, IISER Bhopal, India
Jack Clegg, University of Queensland, Australia
Simon Coles, University of Southampton, UK
Richard Cooper, University of Oxford, UK
Franziska Emmerling, Federal Institute for
Materials Research and Testing in Berlin,
Germany
Paolo Falcaro, TU Graz, Austria
Sylvie Ferlay, Institut Le Bel, France
Antonio Frontera, University of the Balearic
Islands, Spain

Georg Garnweitner, TU Braunschweig,
Germany
David Harding, Walailak University, Thailand
Chris Hawes, University of Keele, UK
Delia Haynes, University of
Stellenbosch, South Africa
Kristin Hutchins, Texas Tech University, USA
Christoph Janiak, University of Dusseldorf,
Germany
Franca Jones, Curtin University, Australia
Bart Kahr, New York University, USA
Andrzej Katrusiak, Adam Mickiewicz
University, Poland
Niveen Khashab, KAUST, Saudi Arabia
Jing Li, Rutgers University, USA
Chiara Maccato, Padova University, Italy
Leonard MacGillivray, University of Iowa, USA
Yuji Matsumoto, Tohoku University, Japan
Sharmarke Mohamed, Khalifa University, UAE
Abel Moreno, National Autonomous University
of Mexico, Mexico

Anja-Verena Mudring, Aarhus University,
Denmark
Parthapratim Munshi, Shiv Nadar University,
India
Ashwini Nangia, University of Hyderabad,
India
Lars Öhrström, Chalmers University of
Technology, Sweden
Simon Parsons, University of Edinburgh, UK
Cynthia Pereira, Universidade Federal de
Minas Gerais-UFMG, Brazil
Concepció Rovira, Institut de Ciència de
Materials de Barcelona, Spain
Calvin Sun, University of Minnesota, USA
Wei-Yin Sun, Nanjing University, China
Jennifer Swift, Georgetown University, USA
Edward R T Tiekink, Sunway University,
Malaysia
Ali Trabolsi, NYU Abu Dhabi, UAE
Hongjie Zhang, Changchun Institute of
Applied Chemistry, China

Information for Authors

Full details on how to submit material for publication in
CrystEngComm are given in the Instructions for Authors (available
from <http://www.rsc.org/authors>). Submissions should be made via the
journal's homepage: rsc.li/crystengcomm. Submissions: The journal
welcomes submissions of manuscripts for publication as Full Papers,
Communications and Highlights. Full Papers and Communications
should describe original work of high quality and impact on the design
and understanding of crystalline materials. We welcome studies that
highlight the novel properties or applications (or potential properties/
applications) of the materials studied.

Authors may reproduce/republish portions of their published
contribution without seeking permission from the Royal Society of
Chemistry, provided that any such republication is accompanied by
an acknowledgement in the form: (Original Citation)–Reproduced by
permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2022.

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 Regulation 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 Publishers 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.

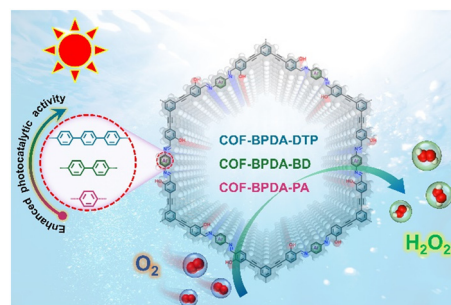
Registered charity number: 207890



4511

Linker length-dependent hydrogen peroxide photosynthesis performance over crystalline covalent organic frameworks

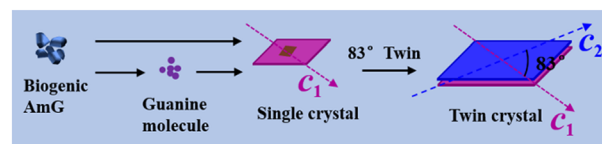
Tao Yang, Yingchu Wang, Yue Chen, Xueqing Peng, Hengqiang Zhang* and Aiguo Kong*



4521

Formation mechanism of twinned β -form anhydrous guanine platelets in scallop eyes

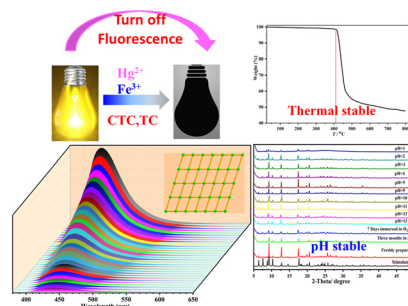
Dongmei Guo, Yiqun Liu, Xiubin Hou, Xubo Wang, Cheng Fan, Lixia Bao, Xinpeng He, Hongmei Zhang and Yurong Ma*



4531

A highly thermal and pH-stable fluorescence sensor for rapid detection of Hg^{2+} , Fe^{3+} , and tetracycline in aqueous solutions

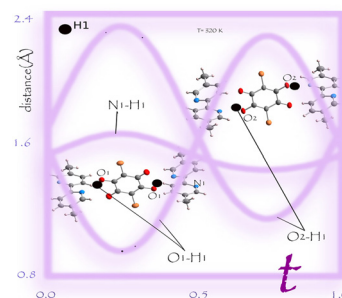
Xuancheng Sun, Chaoxiong Li, Xianggao Meng,* Dunjia Wang and Chunyang Zheng*



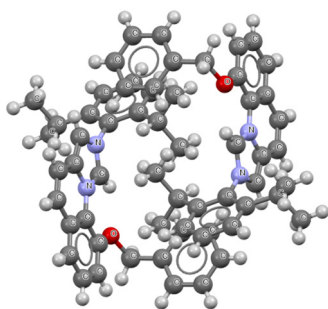
4539

Superspace approach helps: determination of proton dynamics in the phase transition of modulated supramolecular ferroelectrics: 5,5'-dimethyl-2,2'-bipyridine and bromanilic acid

Leila Noohinejad,* Sander van Smaalen, Carsten Paulmann and Martin Tolkiehn



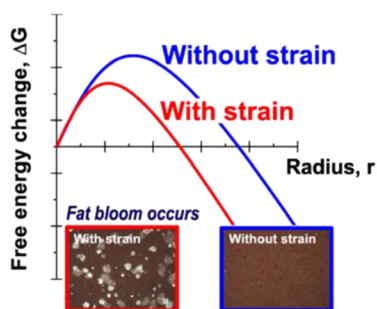
4550



C–H⋯C hydrogen bond and alkali metal C⋯Z⋯C (Z = Li, Na, K) analogues – *N*-heterocyclic carbenes in coordination spheres of protons and alkali metal cations: crystal structures and theoretical analysis

Stawomir J. Grabowski*

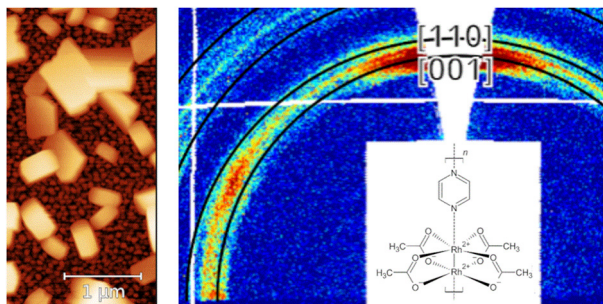
4562



Effect of accumulated strain on fat bloom in CBS-based compound chocolates

Haruhiko Koizumi,* Kazuki Kimura, Mayuko Takagi, Soichi Michikawa, Yuta Hirai, Kiyotaka Sato and Satoru Ueno

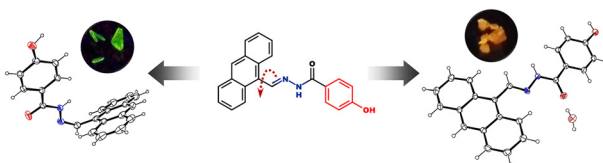
4568



Morphology and orientation change of layer-by-layer deposited one- and two-dimensional coordination polymer nanocrystals containing rhodium paddle-wheel units

Daniel Steinbach, Richard Neubert, Sophie Gersdorf, Christian Schimpf, Denise Erb, David Rafaja, Felix A. Plamper* and Florian Mertens*

4582



Effect of twisted molecular geometry on the solid-state emissions of an anthracene fluorophore

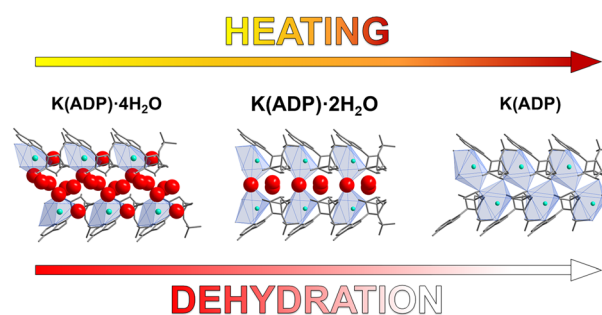
Gayatri Gogoi and Rupam J. Sarma*



4592

Structural aspects of dehydration and rehydration in the adenosine 5'-diphosphate (ADP)–potassium–water system

Oskar Kaszubowski* and Katarzyna Ślepokura



4604

Influence of sapphire substrate with miscut angles on hexagonal boron nitride films grown by halide vapor phase epitaxy

Minghao Chen, Qian Zhang, Chunlei Fang, Zhijie Shen, Yong Lu, Ting Liu,* Shuxin Tan* and Jicai Zhang*

