

# CrystEngComm

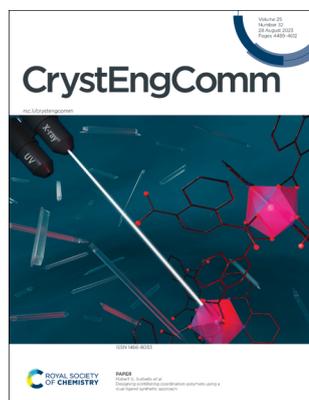
A journal at the forefront of the design and understanding of solid-state and crystalline materials

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

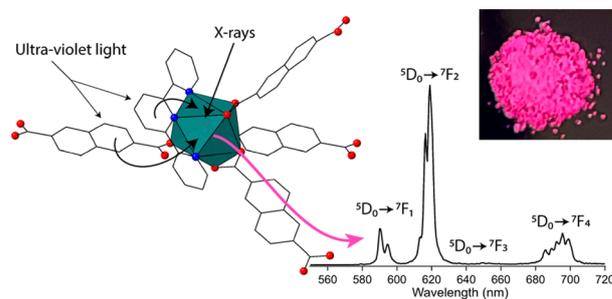
See Robert G. Surbella *et al.*, pp. 4496–4502.  
Image reproduced by permission of Battelle Memorial Institute from *CrystEngComm*, 2023, 25, 4496.

## PAPERS

4496

### Designing scintillating coordination polymers using a dual-ligand synthetic approach

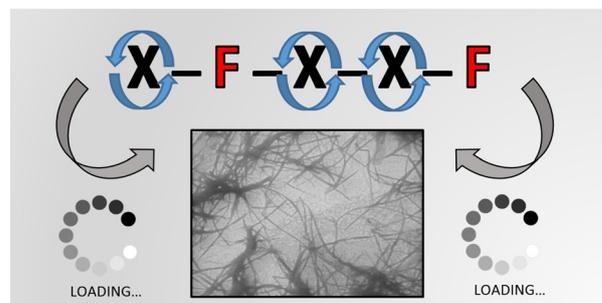
Ana Arteaga, Alice Lulich, May Nyman and Robert G. Surbella III\*



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](mailto:crystengcomm@rsc.org)

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

Email [crystengcomm-rsc@rsc.org](mailto: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](mailto: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](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.

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](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

# CrystEngComm

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

[rsc.li/crystengcomm](http://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  
Concepcio 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](http://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.

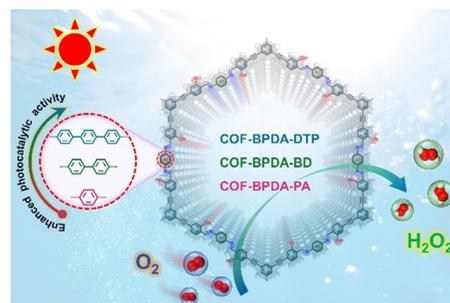
Registered charity number: 207890



4511

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

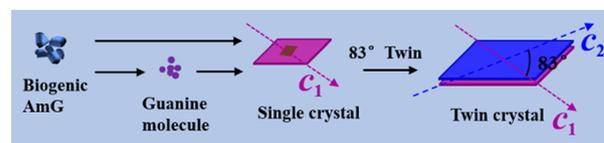
Tao Yang, Yingchu Wang, Yue Chen, Xueqing Peng, Hengqiang Zhang\* and Aiguo Kong\*



4521

### Formation mechanism of twinned $\beta$ -form anhydrous guanine platelets in scallop eyes

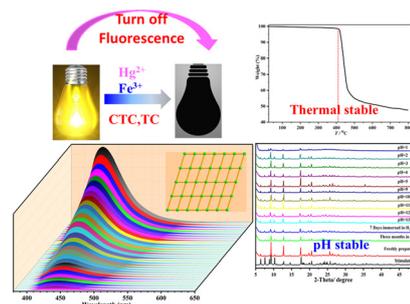
Dongmei Guo, Yiqun Liu, Xiubin Hou, Xubo Wang, Cheng Fan, Lixia Bao, Xinpeng He, Hongmei Zhang and Yurong Ma\*



4531

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

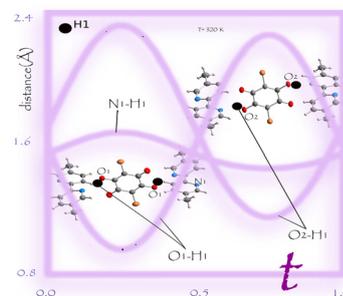
Xuancheng Sun, Chaoxiong Li, Xianggao Meng,\* Dunjia Wang and Chunyang Zheng\*



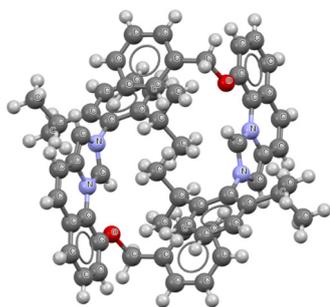
4539

### 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



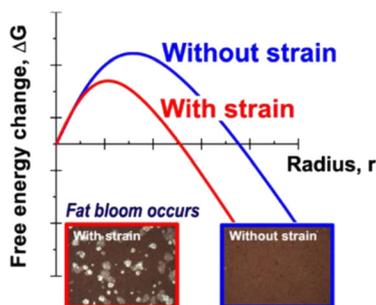
4550



**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\*

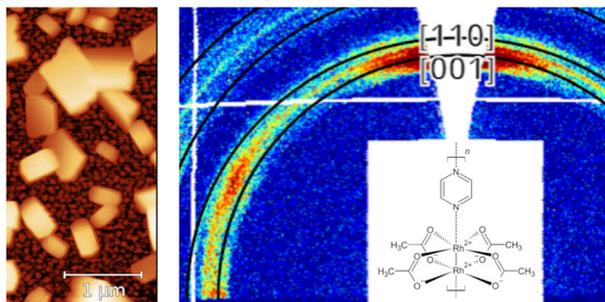
4562



**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

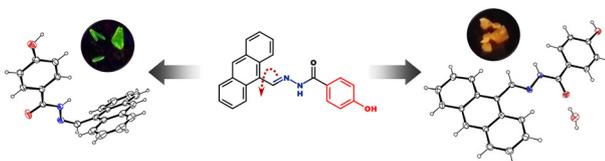
4568



**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**

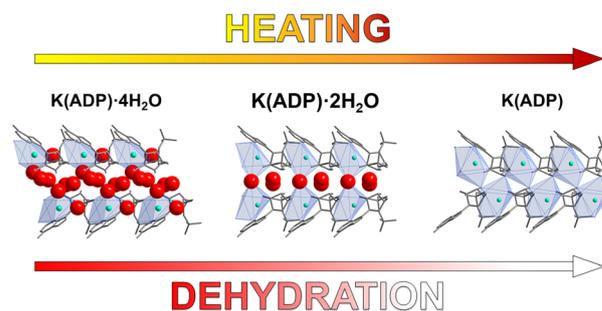
Gayatri Gogoi and Rupam J. Sarma\*



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\*

