

# CrystEngComm

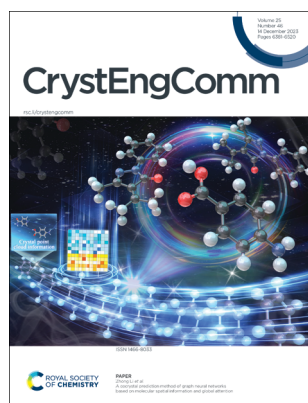
A journal at the forefront of the design and understanding of solid-state and crystalline materials

[rsc.li/crystengcomm](https://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(46) 6381-6520 (2023)



### Cover

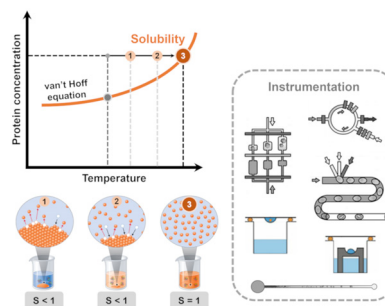
See Zhong Li *et al.*,  
pp. 6405–6415.  
Image reproduced by  
permission of Yanlei Kang  
from *CrystEngComm*, 2023,  
25, 6405.

## HIGHLIGHT

6388

### Advances in protein solubility and thermodynamics: quantification, instrumentation, and perspectives

Joana Ferreira and Filipa Castro\*

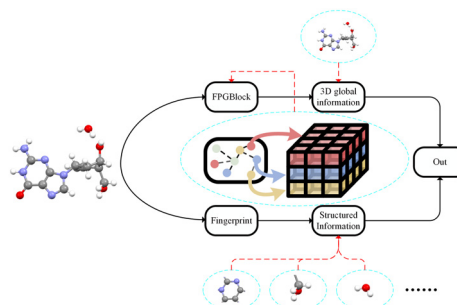


## PAPERS

6405

### A cocrystal prediction method of graph neural networks based on molecular spatial information and global attention

Yanlei Kang, Jiahui Chen, Xiurong Hu, Yunliang Jiang and Zhong Li\*



## Editorial Staff

### Executive Editor

Sally Howells-Wyllie

### Deputy Editor

Mike Andrews

### Development Editors

Michelle Canning, Emily Cuffin-Munday

### 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-Wyllie, 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)

2023 Annual (electronic) subscription price: £1349; US\$2003.  
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

Aurora Cruz-Cabeza, Durham University, UK  
Susan M. Reutzel-Edens, SuRE Pharma  
Consulting, LLC, Zionsville, USA  
Changquan Calvin Sun, University of  
Minnesota, USA  
Bin Zhao, Nankai University, China

## Advisory Board

Christer Aakeroy, Kansas State University, USA  
Srinivasulu Aitipamula, Institute of Chemical  
and Engineering Sciences, Singapore  
Alessia Bacchi, University of Parma, Italy  
Elena Boldyreva, Novosibirsk State University,  
Russia  
Andrew Bond, University of Cambridge, UK  
Deepak Chopra, IISER Bhopal, India  
Jack Clegg, University of Queensland, Australia  
Simon Coles, University of Southampton, UK  
Franziska Emmerling, Federal Institute for  
Materials Research and Testing in Berlin,  
Germany  
Paolo Falcaro, TU Graz, Austria  
Omar Farha, Northwestern University, USA  
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  
Jing Li, Rutgers University, USA  
Tong-Bu Lu, Tianjin University of Technology,  
China  
Chiara Maccato, Padova University, Italy  
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  
Wei-Yin Sun, Nanjing University, China  
Jennifer Swift, Georgetown University, USA  
Edward R T Tieckink, Sunway University,  
Malaysia  
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 2023.

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

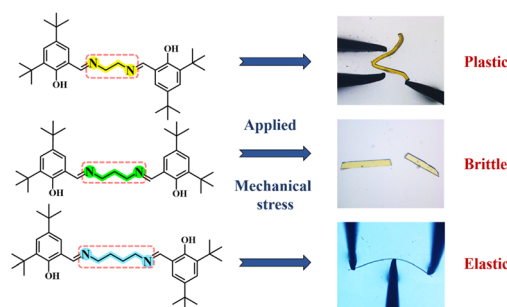


## PAPERS

6416

## Linker size dependent mechanical properties of diimine based molecular crystals

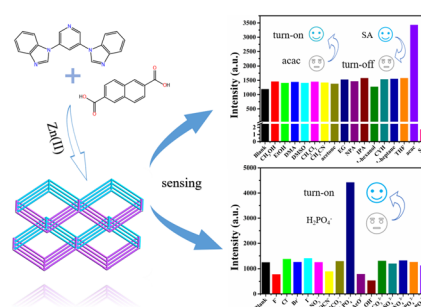
Deepak Manoharan, Shamim Ahmad, Srinu Tothadi, Franziska Emmerling, Biswajit Bhattacharya\* and Soumyajit Ghosh\*



6424

2D → 3D polycatenated Zn(II) metal–organic framework with good chemical stability as a fluorescent sensor toward salicylaldehyde, acetylacetone and  $\text{H}_2\text{PO}_4^-$ 

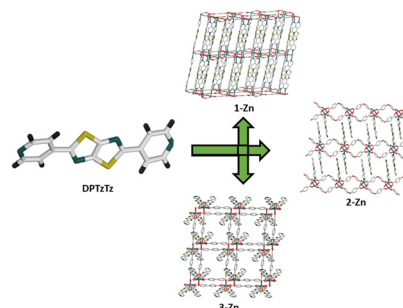
Ya-Ping Li,\* Jian-Hua Zhang, Xiao-Xia Zhang and Sui-Jun Liu\*



6434

The physical and electronic properties of Metal–Organic Frameworks containing dipyrldithiazolo[5,4-*d*]thiazole

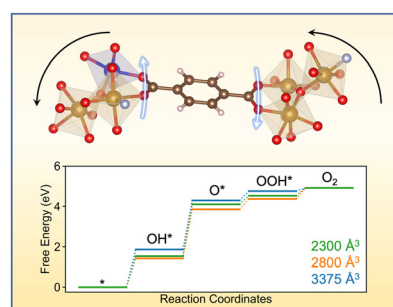
Felix J. Rizzuto, Shyam C. Pal, Eleanor R. Kearns, Carol Hua, Marcello B. Solomon, Patrick W. Doheny, Thomas B. Faust, Cameron J. Kepert,\* Madhab C. Das\* and Deanna M. D'Alessandro\*



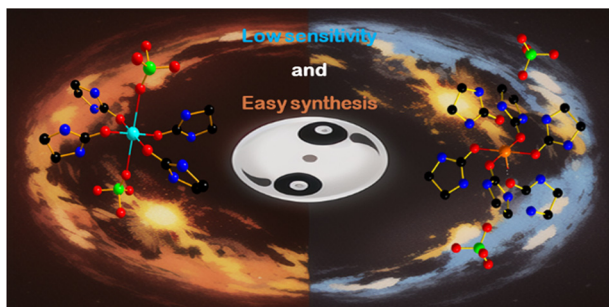
6441

## Catalytic activities modulated by flexible bimetallic metal–organic frameworks

Xiang He\*



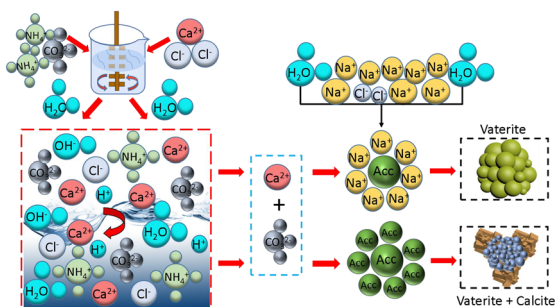
6449



## 2-Imidazolidone metal complexes: increased hydrogen bonds and fused ring ligand ratio to be insensitive

Baolong Kuang,\* Tingwei Wang,\* Chao Zhang, Han Zhang, Zujia Lu, Zhiming Xie, Meiqi Xu, Zhenxin Yi and Jianguo Zhang\*

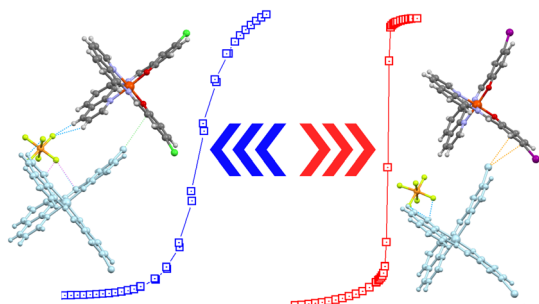
6455



## Influence of Na<sup>+</sup> on vaterite formation, content and yield using steamed ammonia liquid waste as a calcium source

Xuwen Song,\* Xinrui Hua, Xiaomin Zhang,\* Yuxin Tuo, Yihan Su, Jianxiang Ma,\* Sicheng Mu, Tianxing Chen, Panyang He, Lianjing Ma and Cunjian Weng\*

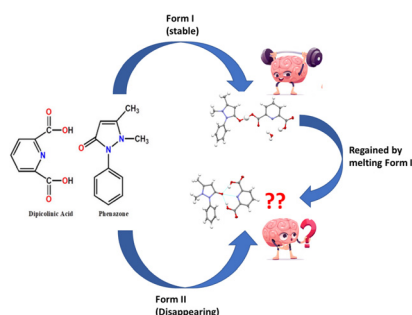
6472



## Structural features that modulate the sharpness of the spin crossover transition in [Fe<sup>III</sup>(5-X-qsal)<sub>2</sub>]<sup>+</sup> based salts

Bruno J. C. Vieira,\* Laura C. J. Pereira,\* Vasco da Gama and João C. Waerenborgh

6478



## In the pursuit of a ‘disappearing’ anhydrous phase of the antipyrine–dipicolinic acid (ANT–DPA) co-crystal: explained through relative stability and charge density analyses

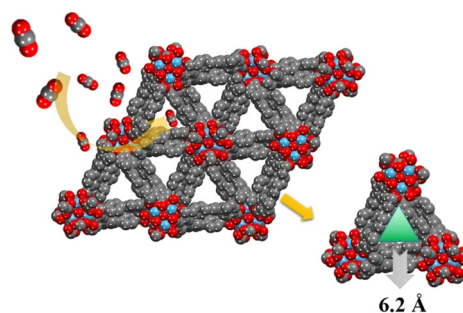
Sehrish Akram, Arshad Mehmood,\* Sajida Noureen and Maqsood Ahmed\*



6489

### A stable ultra-microporous hafnium-based metal-organic framework with high performance for CO<sub>2</sub> adsorption and separation

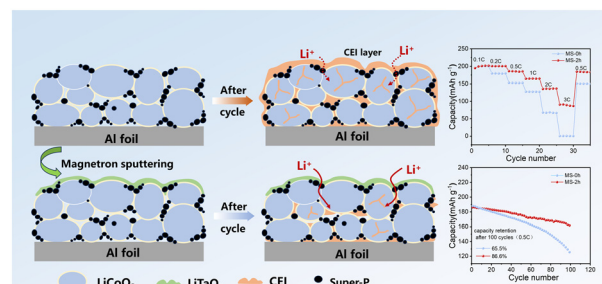
Yali Ma, Haitang Wang, Hailong Wang, Jiani Wang, Shuaiyu Jiang, Qiang Zheng, Songyan Jia, Xue Li\* and Tianyi Ma\*



6496

### The improvement of the high voltage performance of LiCoO<sub>2</sub> by coating LiTaO<sub>3</sub> via magnetron sputtering

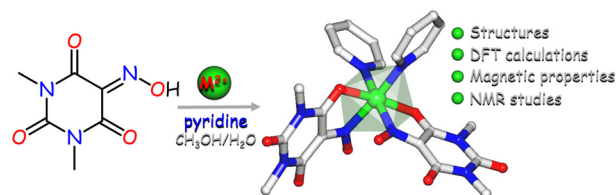
Chenhui Wang, Shaopeng Li, Weiye Chen, Yining Zhao, Shu Xu, Hui Dou and Xiaogang Zhang\*



6503

### Two isostructural complexes of Ni(II) and Zn(II) with violurate and pyridine: a detailed structural, theoretical, magnetic, and NMR investigation

Subhadip Roy, Susital Mal, Rupak Banik, Subrata Das,\* Ľubor Dlhán, Ján Titiš,\* Roman Boča, Alexander M. Kirillov,\* Alexander S. Novikov, Paul Hazendonk,\* Ray J. Butcher, Antonio Bauza and Antonio Frontera\*



6512

### Microwave-assisted hydrothermal solution process for accelerated formation of 3D hierarchical flowery anatase-TiO<sub>2</sub> microspheres with excellent photocatalytic activity

Praveen Kumar Lavudya, SuryaBindu Sesha Devarakonda, Harita Pant, Sarah Geo, Avijit Tudu, Vadali Venkata Satya Siva Srikanth and Rajanikanth Ammanabrolu\*

