

CrystEngComm

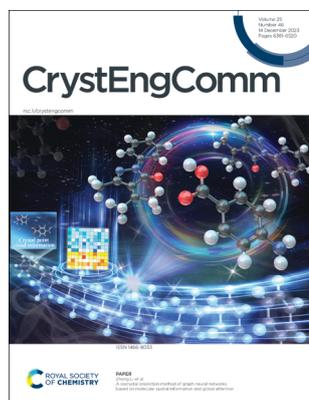
A journal at the forefront of the design and understanding of solid-state and crystalline materials

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(46) 6381-6520 (2023)



Cover

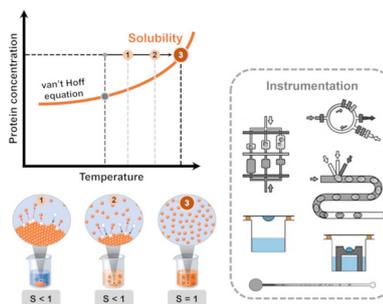
See Zhong Li *et al.*, pp. 6405–6415.
Image reproduced by permission of Yanlei Kang from *CrystEngComm*, 2023, 25, 6405.

HIGHLIGHT

6388

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

Joana Ferreira and Filipa Castro*

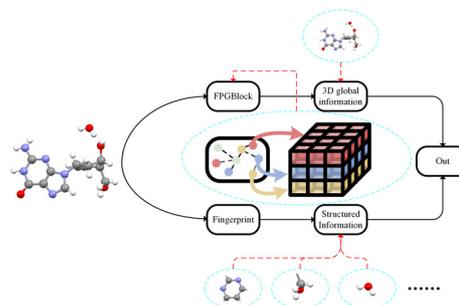


PAPERS

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

For pre-submission queries please contact

Sally Howells-Wyllie, 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

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

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

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 Tiekink, 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. 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.

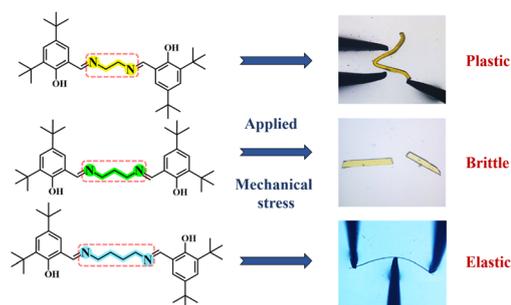
Registered charity number: 207890



6416

Linker size dependent mechanical properties of diimine based molecular crystals

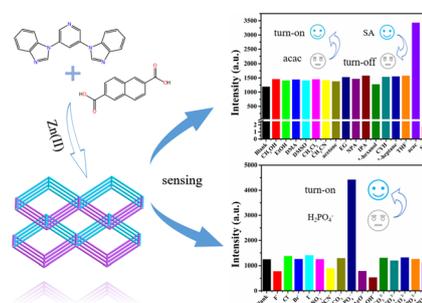
Deepak Manoharan, Shamim Ahmad, Srinu Tothadi, Franziska Emmerling, Biswajit Bhattacharya* and Soumyajit Ghosh*



6424

2D → 3D polycatenated Zn(II) metal-organic framework with good chemical stability as a fluorescent sensor toward salicylaldehyde, acetylacetone and H₂PO₄⁻

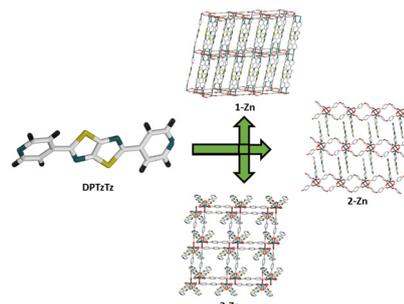
Ya-Ping Li,* Jian-Hua Zhang, Xiao-Xia Zhang and Sui-Jun Liu*



6434

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

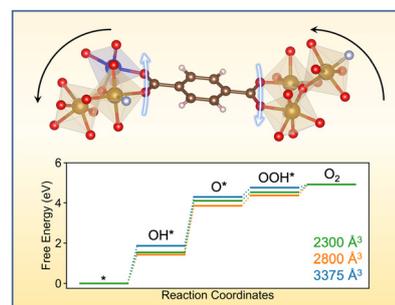
Felix J. Rizzuto, Shyam C. Pal, Eleanor R. Kearns, Carol Hua, Marcello B. Solomon, Patrick W. Doheny, Thomas B. Faust, Cameron J. Kepert,* Madhab C. Das* and Deanna M. D'Alessandro*



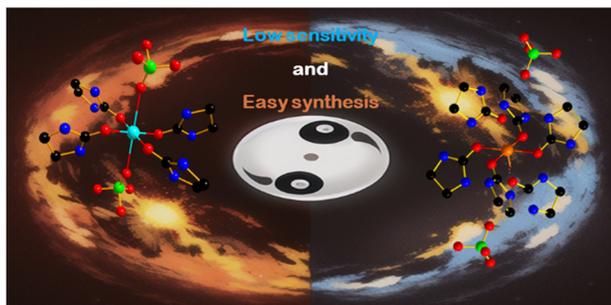
6441

Catalytic activities modulated by flexible bimetallic metal-organic frameworks

Xiang He*



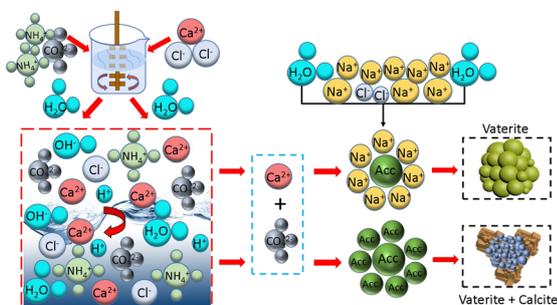
6449



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*

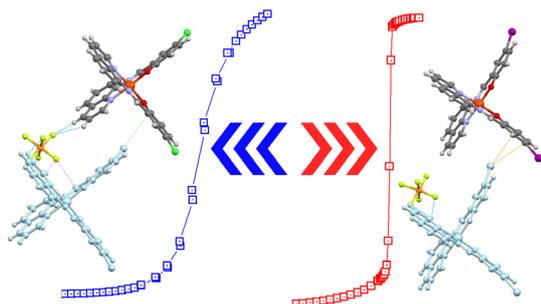
6455



Influence of Na⁺ 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*

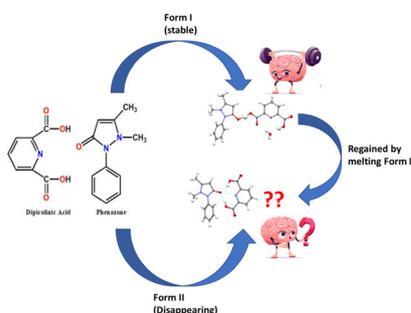
6472



Structural features that modulate the sharpness of the spin crossover transition in [Fe^{III}(5-X-qsal)₂]⁺ 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

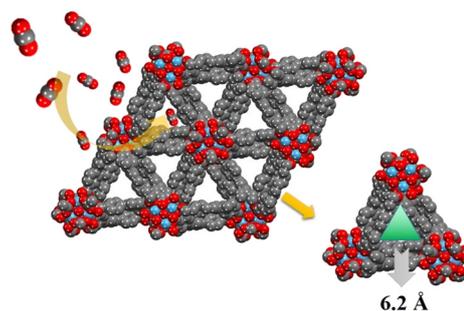
Sehrish Akram, Arshad Mehmood,* Sajida Noureen and Maqsood Ahmed*



6489

A stable ultra-microporous hafnium-based metal-organic framework with high performance for CO₂ adsorption and separation

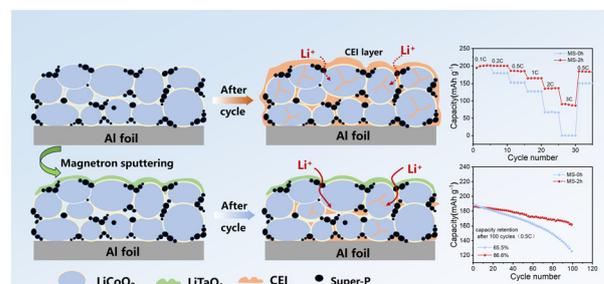
Yali Ma, Haitang Wang, Hailong Wang, Jiani Wang, Shuaiyu Jiang, Qiang Zheng, Songyan Jia, Xue Li* and Tianyi Ma*



6496

The improvement of the high voltage performance of LiCoO₂ by coating LiTaO₃ via magnetron sputtering

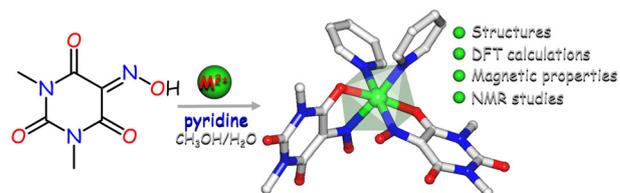
Chenhui Wang, Shaopeng Li, Weiyi Chen, Yining Zhao, Shu Xu, Hui Dou and Xiaogang Zhang*



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,* Lubor 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-TiO₂ microspheres with excellent photocatalytic activity

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

