

# MSDE

## Molecular Systems Design & Engineering rsc.li/molecular-engineering

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 2058-9689 CODEN MSDEBG 8(5) 553-692 (2023)



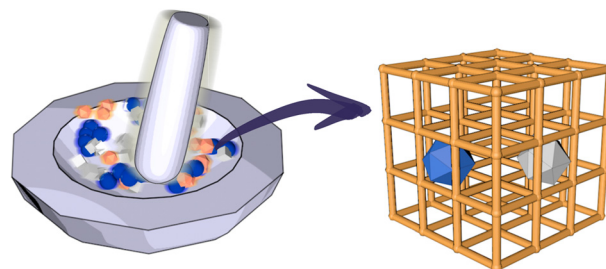
**Cover**  
See Mario Wriedt *et al.*,  
pp. 580–585.  
Image reproduced by  
permission of Mario Wriedt  
from *Mol. Syst. Des. Eng.*,  
2023, 8, 580.

### REVIEW

560

#### Metal–organic framework composites from a mechanochemical process

Wupeng Wang, Milton Chai,\*  
Muhammad Yazid Bin Zulkifli, Kaijie Xu, Yuelei Chen,  
Lianzhou Wang, Vicki Chen and Jingwei Hou\*

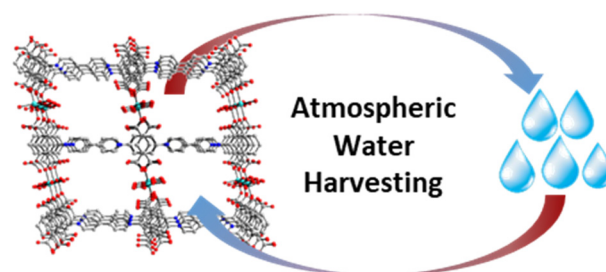


### COMMUNICATIONS

580

#### Water harvesting properties of a zwitterionic metal–organic framework

Charlene C. VanLeuven, Juby R. Varghese, Monu Joy,  
Fletcher B. Dix, Kyle Duell, Donald Hartman  
and Mario Wriedt\*



## Editorial Staff

### Executive Editor

Maria Southall

### Deputy Editor

Bianca Provost

### Editorial Production Manager

Emily Skinner

### Assistant Editors

Sean Browner, Molly Colgate, Paul Scott, Alison Winder

### Editorial Assistant

Basita Javeed

### Publishing Assistant

Allison Holloway

### Publisher

Sam Keltie

For queries about submitted papers, please contact

Emily Skinner, Editorial Production Manager in the first instance.

E-mail: [molecularengineering@rsc.org](mailto:molecularengineering@rsc.org)

For pre-submission queries please contact

Maria Southall, Executive Editor.

E-mail: [molecularengineering-rsc@rsc.org](mailto:molecularengineering-rsc@rsc.org)

MSDE (electronic: ISSN 2058-9689) is published 12 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: £2211; \$3649.

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)

# MSDE

Molecular Systems Design & Engineering

[rsc.li/molecular-engineering](http://rsc.li/molecular-engineering)

Building and designing systems from the molecular level

## Editorial Board

### Chair

Juan de Pablo, University of Chicago, USA

### Associate Editors

Luke Connal, Australian National University, Australia

Robert Riggleman, University of Pennsylvania, USA

### Members

Claire S. Adjiman, Imperial College London, UK

Linda Broadbelt, Northwestern University, USA

Andrew Ferguson, University of Chicago, USA

LaShanda Korley, University of Delaware, USA

Yongye Liang, Southern University of Science and Technology, China

Anja Palmans, Eindhoven University of Technology, The Netherlands

Patrick Stayton, University of Washington, USA

## Advisory Board

Alfredo Alexander-Katz, MIT, USA

Helena Azevedo, Queen Mary University of London, UK

Andre Bardow, ETH Zurich, Switzerland

Jeremy Baumberg, University of Cambridge, UK

Joao Cabral, Imperial College London, UK

Neil Champness, University of Nottingham, UK

Paulette Clancy, John Hopkins University, USA

Marc-Olivier Coppens, UCL, UK

Graeme Day, University of Southampton, UK

Andrew deMello, ETH Zurich, Switzerland

Cecile Dreiss, Kings College London, UK

Thomas Epps III, University of Delaware, USA

Lei Fang, Texas A&M University, USA

C. Daniel Frisbie, University of Minnesota, USA

Xuefeng Guo, Peking University, China

Kristi Kiick, University of Delaware, USA

Raju Kumar Gupta, Indian Institute of Technology

Kanpur, India

Sarah Heilshorn, Stanford University, USA

Arthi Jayaraman, University of Delaware, USA

Takashi Kato, University of Tokyo, Japan

Sang Ouk Kim, KAIST, Republic of Korea

Jodie Lutkenhaus, Texas A&M University, USA

Heidi Mansour, University of Arizona, USA

Bert Meijer, Eindhoven University of Technology,

Netherlands

Takashi Nakanishi, NIMS, Japan

Ki Tae Nam, Seoul National University, Republic

of Korea

Insup Noh, Seoul National University of Science &

Technology, Republic of Korea

Mark A. Olson, Tianjin University, China

Ho Bum Park, Hanyang University,

South Korea

Jon Parquette, Ohio State University, USA

Boaz Pokroy, Technion – Israel Institute of

Technology, Israel

Jeffrey Rimer, University of Houston, USA

Shu Seki, Kyoto University, Japan

Randy Snurr, Northwestern University, USA

Brigitte Stadler, Aarhus University, Denmark

Doros Theodorou, National Technical University of

Athens, Greece

Matthew Tirrell, University of Chicago, USA

Bernhardt L. Trout, MIT, USA

Raymond W. Y. Wong, Hong Kong

Polytechnic University, Hong Kong

Jia Zhu, Nanjing University, China

Meifang Zhu, Donghua University, China

## Information for Authors

Full details on how to submit material for publication in MSDE 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/molecular-engineering](http://rsc.li/molecular-engineering). Submissions: The journal welcomes submissions of manuscripts for publication as Review Articles and Minireviews. Full Papers and Communications should describe original work of high quality and impact.

Additional details are available from the Editorial Office or <http://www.rsc.org/authors>

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.

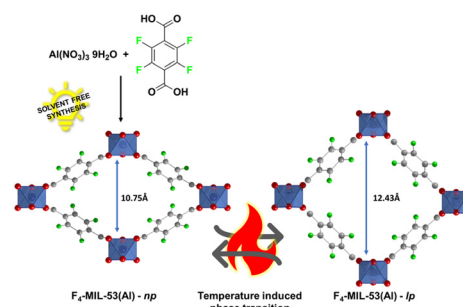
Registered charity number: 207890



586

### Solvent-free synthesis of a new perfluorinated MIL-53(Al) with a temperature-induced breathing effect

Diletta Morelli Venturi, Virginia Guiotto, Roberto D'Amato, Lucia Calucci, Matteo Signorile, Marco Taddei, Valentina Crocellà\* and Ferdinando Costantino\*

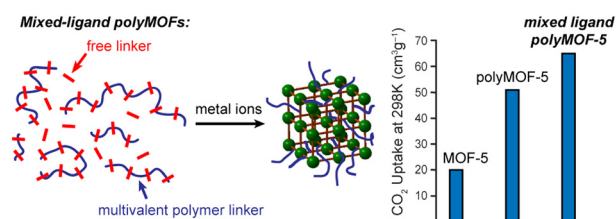


## PAPERS

591

### Mixing ligands to enhance gas uptake in polyMOFs

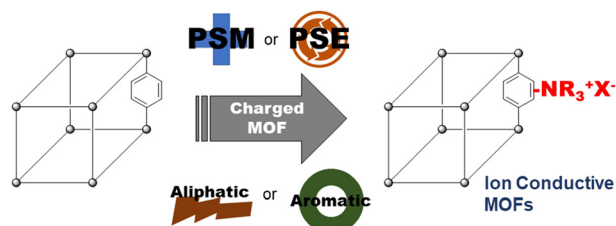
Matthew A. Pearson, Sachin Bhagchandani, Mircea Dincă and Jeremiah A. Johnson\*



598

### Efficient and strategical installations of quaternary ammonium groups in metal-organic frameworks for hydroxide conductivity

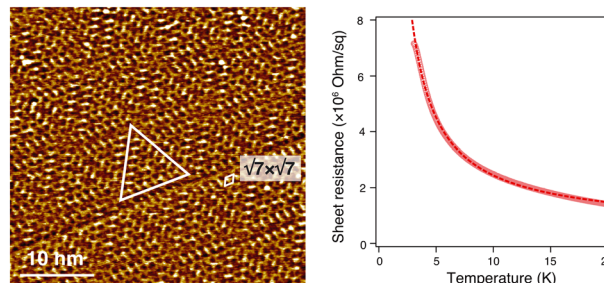
Ho Jeong Choi, Seungpyo Hong, Younghu Son, Ki Tae Kim, Cheoljae Kim, Minyoung Yoon\* and Min Kim\*



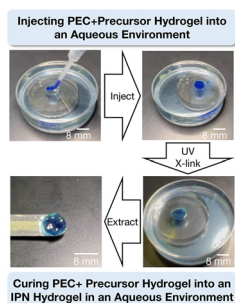
604

### Few-monolayer Ga film on Si(111): illusive gallene formation and localization instead of superconductivity

L. V. Bondarenko, A. Y. Tupchaya, Y. E. Vekovshinin, D. V. Gruznev, A. N. Mihalyuk, D. V. Denisov, A. V. Matetskiy, D. A. Olyanich, T. V. Utas, V. S. Zhdanov, A. V. Zotov and A. A. Saranin\*



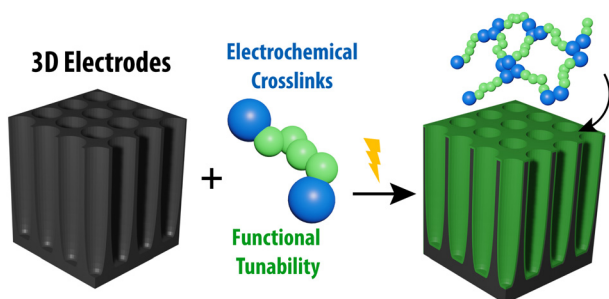
611



### Polyelectrolyte complex scaffoldings for photocrosslinked hydrogels

Defu Li, Mahsa Ghowvati, Nasim Annabi and Samanvaya Srivastava\*

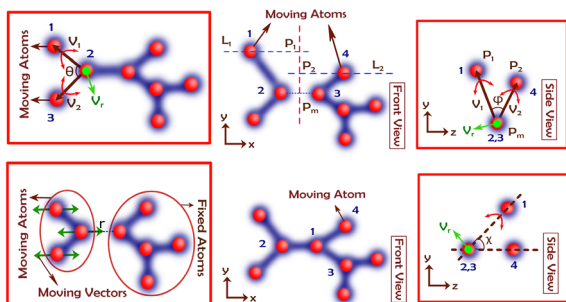
624



### Conformal electrodeposition of ultrathin polymeric films with tunable properties from dual-functional monomers

Wenlu Wang, Zhaoyi Zheng, Anton B. Resing, Keith A. Brown and Jörg G. Werner\*

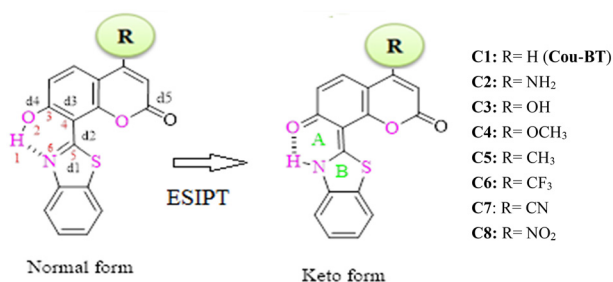
632



### A computational framework for evaluating molecular dynamics potential parameters employing quantum mechanics

Amirmasoud Lanjan, Zahra Moradi and Seshasai Srinivasan\*

647



### TD-DFT study of the excited state intramolecular proton transfer (ESIPT) mechanism and photophysical properties in coumarin-benzothiazole derivatives: substitution and solvent effects

Hossein Roohi\* and Tahereh Pouryahya



666

### Combining multi-scale simulations and experiments to unveil the adsorption of methylene blue in graphene tridimensional-based materials

Mayara B. Leão, Laura F. O. Vendrame, Solange B. Fagan, Ivana Zanella, Iuri M. Jauris, José R. Bordin and Carolina F. de Matos\*



681

### On-surface polymerisation and self-assembly of DPP-based molecular wires

Michael Clarke, Abigail Bellamy-Carter, Ferdinando Malagrecia, Jack Hart, Stephen P. Argent, James N. O'Shea, David B. Amabilino and Alex Saywell\*

