# **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(6) 693-824 (2023)



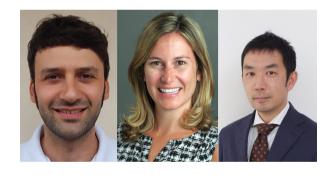
#### Cover See Florian Glöcklhofer et al., pp. 713-720. Image reproduced by permission of Florian Glöcklhofer from Mol. Syst. Des. Eng., 2023, 8, 713.

#### **EDITORIAL**

700

# Introduction to molecular engineering in MOFs: beyond reticular chemistry

Marco Taddei, Ashlee J. Howarth and Takashi Uemura

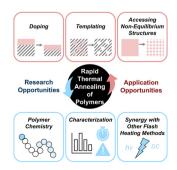


# **REVIEW**

701

# Recent advances and emerging opportunities in rapid thermal annealing (RTA) of polymers

Reika Katsumata,\* Claire Senger and James Nicolas Pagaduan



#### **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

For pre-submission queries please contact Maria Southall, Executive Editor. E-mail: 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

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

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:

Advertisement sales:

Telephone: +44 (0) 207 4378 6556.

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

# **MSDE**

Molecular Systems Design & Engineering 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, Memhers

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

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

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
RaymondW.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. 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

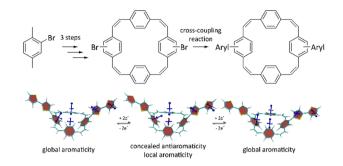


# **PAPERS**

# 713

Functionalisation of conjugated macrocycles with type I and II concealed antiaromaticity via crosscoupling reactions

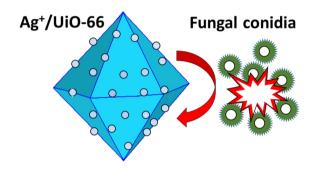
Troy L. R. Bennett, Adam V. Marsh, James M. Turner, Felix Plasser, Martin Heeney and Florian Glöcklhofer\*



#### 721

Nanosilver-loaded metal-organic framework UiO-66 with strong fungicidal activity

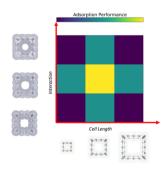
Carolina Chiericatti, Luis A. Lozano and Juan M. Zamaro\*



# 733

Molecular understanding of the impacts of structural characteristics on ethanol adsorption performance for adsorption heat pumps

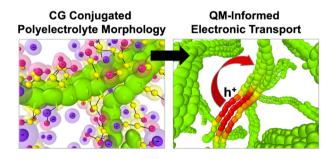
Wei Li, Zhilu Liu, Weixiong Wu and Song Li\*



#### 743

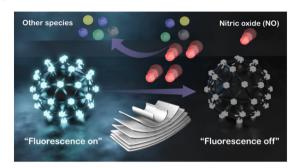
Electron and ion transport in semi-dilute conjugated polyelectrolytes: view from a coarsegrained tight binding model

David M. Friday and Nicholas E. Jackson\*



# **PAPERS**

#### 756



# Post engineering of a chemically stable MOF for selective and sensitive sensing of nitric oxide

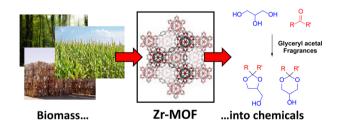
Writakshi Mandal, Dipanjan Majumder, Sahel Fajal, Sumanta Let, Mandar M. Shirolkar and Sujit K. Ghosh\*

767



Substituent effect on controlled release of fragrant aldehydes from pH-triggered nicotinoylhydrazonebased precursors

Zuobing Xiao, Chengjing Wu, Xinyu Lu,\* Yunwei Niu, Peiran Yu and Xiaojie Ma



Zr-containing UiO-66 metal-organic frameworks as efficient heterogeneous catalysts for glycerol valorization: synthesis of hyacinth and other glyceryl acetal fragrances

A. Rapeyko,\* J. C. Díaz Infante and F. X. Llabrés i Xamena\*



In silico study of the binding of daunomycin and phenylalanine transfer RNA: probe molecular recognition for structure-based drug design

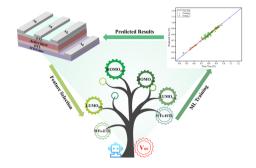
Gonghao Wu, Jipeng Li, Jianxin Yang\* and Xingqing Xiao\*

# **PAPERS**

# 799

Machine learning assisted identification of the matched energy level of materials for high open circuit voltage in binary organic solar cells

Kuo Wang, Chaorong Guo, Zhennan Li, Rui Zhang, Zhimin Feng, Gengkun Fang, Di Huang,\* Jiaojiao Liang,\* Ling Zhao\* and Zicha Li



#### 810

Peripherally and non-peripherally carboxylic acid substituted Cu(II) phthalocyanine/reduced graphene oxide nanohybrids for hydrogen evolution reaction catalysts

Ekrem Kaplan, Tolga Karazehir, Selin Gümrükçü, Baran Sarac, A. Sezai Sarac and Esin Hamuryudan\*

