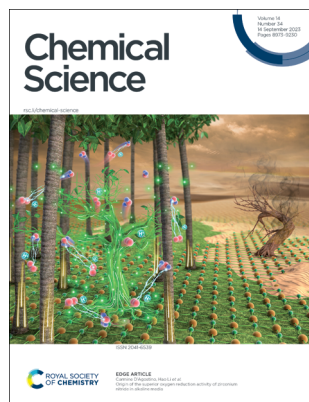


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(34) 8973–9230 (2023)



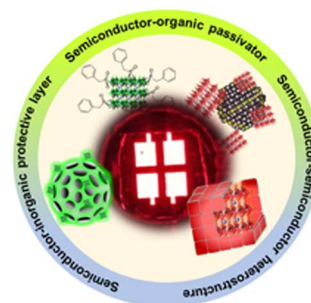
**Cover**  
See Carmine D'Agostino, Hao Li *et al.*, pp. 9000–9009. Image reproduced by permission of Hao Li from *Chem. Sci.*, 2023, **14**, 9000.

## PERSPECTIVE

8984

### Impact of core–shell perovskite nanocrystals for LED applications: successes, challenges, and prospects

Samrat Das Adhikari, Andrés F. Gualdrón Reyes, Subir Paul, Jeevan Torres, Beatriu Escuder, Iván Mora-Seró and Sofia Masi\*

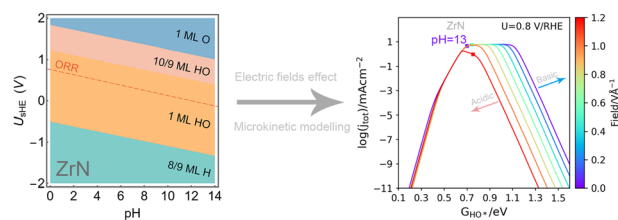


## EDGE ARTICLES

9000

### Origin of the superior oxygen reduction activity of zirconium nitride in alkaline media

Heng Liu, Di Zhang, Stuart M. Holmes, Carmine D'Agostino\* and Hao Li\*



## Editorial Staff

### Executive Editor

May Copsy

### Deputy Editor

Samantha Apps

### Senior Editor

James Moore

### Scientific Editors

Ellis Crawford, Jingtao Huang, Esther Johnston, Sophie Orchard, Richard Thompson and Amy Welch

### Editorial Assistant

Karina Webster

### Publishing Assistant

David Bishop

For queries about submitted articles please contact James Moore, Senior Editor, in the first instance. E-mail [chemicalscience@rsc.org](mailto:chemicalscience@rsc.org)

For pre-submission queries please contact May Copsy, Executive Editor. E-mail [chemicalscience-rsc@rsc.org](mailto:chemicalscience-rsc@rsc.org)

Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read.

Please email [orders@rsc.org](mailto:orders@rsc.org) to register your interest or contact 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)

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)

# Chemical Science

[rsc.li/chemical-science](http://rsc.li/chemical-science)

## Editorial Board

### Editor-in-Chief

Andrew Cooper, University of Liverpool

### Associate Editors

Vincent Artero, CEA-Grenoble  
Luis M. Campos, Columbia University  
Michelle Chang, University of California, Berkeley  
Lin X. Chen, Northwestern University  
Graeme Day, University of Southampton  
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Mircea Dincă, MIT

François Gabbai, Texas A&M University  
Subi George, JNCASR  
Ryan Gilmour, WWU Münster  
Jinlong Gong, Tianjin University  
Stephen Goldup, University of Birmingham  
Zaiping Guo, University of Adelaide  
Christopher A. Hunter, University of Cambridge  
Malika Jefferies-EL, Boston University  
Ning Jiao, Peking University  
Tanja Junkers, Monash University

Hemamala Karunadasa, Stanford University  
Maja Köhn, University of Freiburg  
Yi-Tao Long, Nanjing University  
Gabriel Merino, CINVESTAV Merida  
James K. McCusker, Michigan State University  
Thomas Meade, Northwestern University  
Paolo Melchiorre, University of Bologna  
Carsten Schultz, Oregon Health & Science University  
Dmitri Talapin, The University of Chicago  
Toshiharu Teranishi, Kyoto University  
Andrei Yudin, University of Toronto

## Advisory Board

Dave Adams, University of Glasgow  
Ayyappanpillai Ajayaghosh, NIIST  
Ulf-Peter Apfel, Ruhr-University Bochum  
Polly Arnold, University of California, Berkeley  
Xinhe Bao, Dalian Institute of Chemical Physics  
Zhenan Bao, Stanford University  
Gonçalo Bernardes, University of Cambridge  
Frank Biedermann, Karlsruhe Institute of Technology  
Donna Blackmond, Scripps Research Institute  
Jeffrey Bode, ETH Zurich  
Jennifer S. Brodbelt, University of Texas at Austin, USA  
Christopher Chang, University of California, Berkeley  
Chi-Ming Che, University of Hong Kong  
Jun Chen, Nankai University  
R. Graham Cooks, Purdue University  
Christophe Copéret, ETH Zurich  
Eugenio Coronado, University of Valencia  
Leroy Cronin, University of Glasgow  
James Crowley, University of Otago  
Christopher C. Cummins, Massachusetts Institute of Technology  
Ben Davis, University of Oxford  
Jillian Dempsey, University of North Carolina at Chapel Hill  
Kazunari Domen, University of Tokyo  
James Durrant, Imperial College London  
Xinlang Feng, TU Dresden  
Ben Feringa, University of Groningen  
Makoto Fujita, University of Tokyo  
Phillip Gale, University of Technology Sydney  
Song Gao, Peking University  
Jeremiah Gassensmith, University of Texas at Dallas  
Elizabeth Gibson, Newcastle University  
Hubert Girault, EPFL  
Frank Glorius, WWU Münster  
Leticia González, University of Vienna  
Duncan Graham, University of Strathclyde

Vicki Grassian, University of California, San Diego  
Alexis Grimaud, Boston College  
Christian Hackenberger, FMP Berlin  
Buxing Han, Chinese Academy of Sciences  
Christy Haynes, University of Minnesota  
Patrick Holland, Yale University  
Kim Jelfs, Imperial College London  
Yousung Jung, KAIST  
Stephanie Kath-Schorr, University of Cologne  
Takashi Kato, University of Tokyo  
Christopher Kelly, Janssen Research & Development  
Jérôme Lacour, University of Geneva  
Ai-Lan Lee, Heriot-Watt University  
Daniele Leonori, RWTH Aachen University  
Chao-Jun Li, McGill University  
Yi Li, Jilin University  
Mi Hee Lim, KAIST  
Wenbin Lin, University of Chicago  
Kopin Liu, Academia Sinica  
Watson Loh, UNICAMP  
Bettina Lotsch, Max Planck Institute  
Xiong Wen (David) Lou, Nanyang Technological University  
Kazuhiko Maeda, Tokyo Institute of Technology  
Satoshi Maeda, Hokkaido University  
Swadhin Mandal, IISER Kolkata  
Ellen Matson, University of Rochester  
Scott Miller, Yale University  
Daniel Mndiola, University of Pennsylvania  
Wonwoo Nam, Ewha Womans University  
Jonathan Nitschke, University of Cambridge  
Allie Obermeyer, Columbia University  
Martin Oestreich, Technical University of Berlin  
Takashi Ooi, Nagoya University  
Rachel O'Reilly, University of Birmingham  
Oleg Ozerov, Texas A&M University  
Xiulian Pan, Dalian Institute of Chemical Physics  
Nicolas Plumeré, Technical University of

Munich  
Rasmita Raval, University of Liverpool  
Erwin Reisner, University of Cambridge  
Andrea Rentmeister, WWU Münster  
Jeffrey Rinehart, University of California, San Diego  
Stuart Rowan, University of Chicago  
Richmond Sarpong, University of California, Berkeley  
Danielle Schultz, Merck  
Dwight Seferos, University of Toronto  
Oliver Seitz, Humboldt University of Berlin  
Roberta Sessoli, University of Florence  
Kay Severin, Federal Polytechnic School of Lausanne  
Mikiko Sodeoka, RIKEN  
Galo Soler-Illia, Universidad Nacional de San Martin  
David Spring, University of Cambridge  
Brian Stoltz, California Institute of Technology  
Brent Sumrlin, University of Florida  
Raghavan B. Sunoj, IIT Bombay  
Yogesh Surendranath, MIT  
Mizuki Tada, Nagoya University  
Ben Zhong Tang, The Chinese University of Hong Kong  
Zhiyong Tang, National Center for Nanoscience and Nanotechnology  
Christine Thomas, Ohio State University  
He Tian, East China University of Science & Technology  
Zhong-Qun Tian, Xiamen University  
F. Dean Toste, University of California, Berkeley  
Takashi Uemura, University of Tokyo  
Jan van Hest, Radboud University  
Latha Venkataraman, Columbia University  
Chu Wang, Peking University  
Julia Weinstein, University of Sheffield  
Tom Welton, Imperial College London  
Charlotte Williams, University of Oxford  
Vivian Yam, University of Hong Kong  
Qi-Lin Zhou, Nankai University  
Jenny Zhang, University of Cambridge

## Information for Authors

Full details on how to submit material for publication in Chemical Science 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/chemical-science](http://rsc.li/chemical-science)

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.

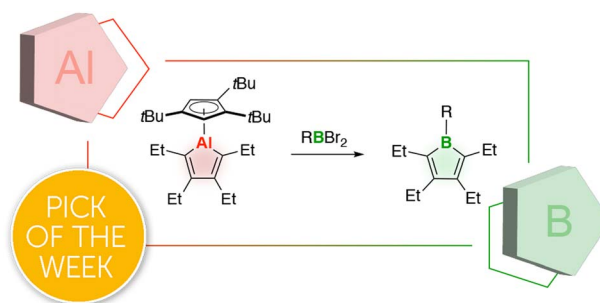
Registered charity number: 207890



9010

### Boroles from alumes: accessing boroles with alkyl-substituted backbones *via* transtrielation

Josina L. Bohlen, Lukas Endres, Regina Drescher, Krzysztof Radacki, Maximilian Dietz, Ivo Krummenacher and Holger Braunschweig\*

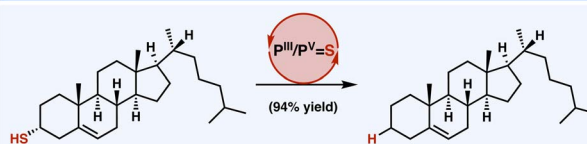


9016

### Metal-free reductive desulfurization of C-sp<sup>3</sup>-substituted thiols using phosphite catalysis

Rana M. I. Morsy, Ganesh Samala, Ankur Jalan, Michael E. Kopach, Naresh M. Venneti\* and Jennifer L. Stockdill\*

#### Metal-Free Reductive Desulfurization by P(III)/P(V) Catalysis



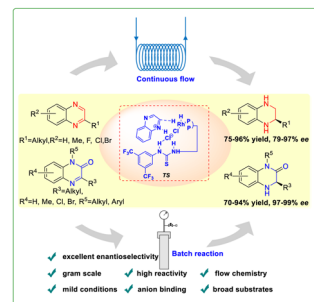
• Good functional group compatibility  
• PhMe and 1,4-dioxane equally effective

• Up to 99% yield  
• No specialized equipment

9024

### Highly enantioselective synthesis of both tetrahydroquinoxalines and dihydroquinoxalinones *via* Rh–thiourea catalyzed asymmetric hydrogenation

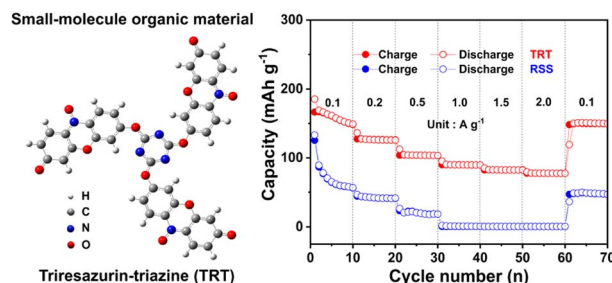
Ana Xu, Chaoyi Li, Junrong Huang, Heng Pang, Chengyao Zhao, Lijuan Song,\* Hengzhi You,\* Xumu Zhang and Fen-Er Chen\*



9033

### Boosting the zinc storage of a small-molecule organic cathode by a desalination strategy

Wei Wang, Ying Tang, Jun Liu, Hongbao Li,\* Rui Wang, Longhai Zhang, Fei Liang, Wei Bai,\* Lin Zhang and Chaofeng Zhang\*

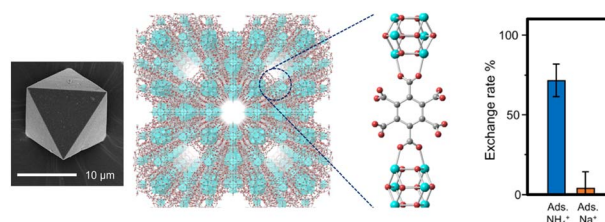




9068

### Design of a robust and strong-acid MOF platform for selective ammonium recovery and proton conductivity

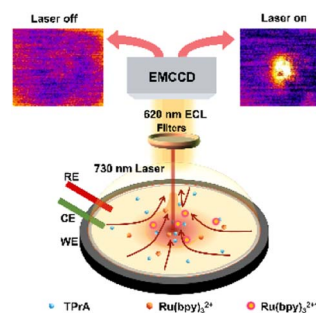
Genki Hatakeyama, Hongyao Zhou, Takashi Kikuchi, Masaki Nishio, Kouki Oka, Masaaki Sadakiyo, Yusuke Nishiyama and Teppei Yamada\*



9074

### Site-selective heat boosting electrochemiluminescence for single cell imaging

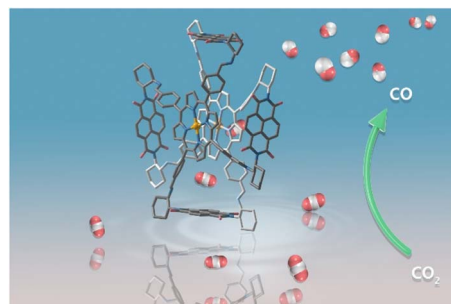
Xiaodan Gou, Yiwen Zhang, Zejing Xing, Cheng Ma,\* Changjie Mao\* and Jun-Jie Zhu\*



9086

### Cofacial porphyrin organic cages. Metals regulating excitation electron transfer and CO<sub>2</sub> reduction electrocatalytic properties

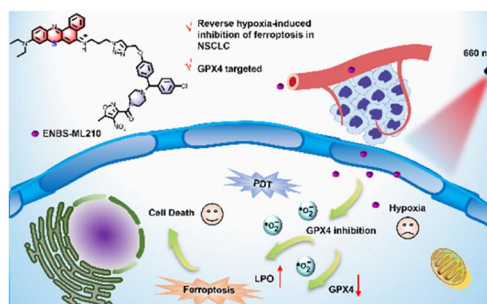
Xiaolin Liu, Chenxi Liu, Xiaojuan Song, Xu Ding, Hailong Wang,\* Baoqiu Yu, Heyuan Liu,\* Bin Han, Xiyou Li\* and Jianzhuang Jiang\*



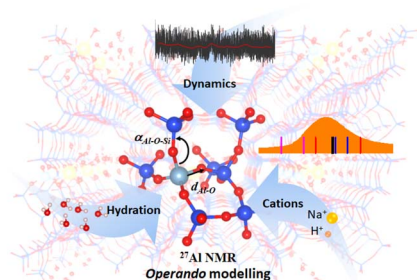
9095

### A GPX4-targeted photosensitizer to reverse hypoxia-induced inhibition of ferroptosis for non-small cell lung cancer therapy

Qiao Hu, Wanjie Zhu, Jianjun Du,\* Haoying Ge, Jiazhu Zheng, Saran Long, Jiangli Fan and Xiaojun Peng



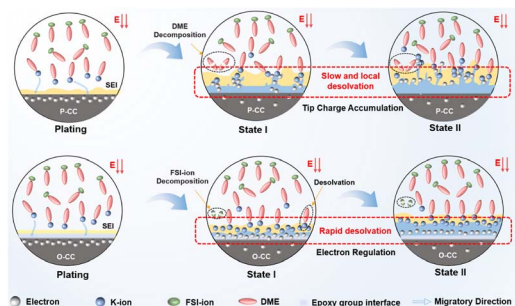
9101



### The need for *operando* modelling of $^{27}\text{Al}$ NMR in zeolites: the effect of temperature, topology and water

Chen Lei, Andreas Erlebach, Federico Brivio, Lukáš Grajciar, Zdeněk Tošner, Christopher J. Heard\* and Petr Nachtigall

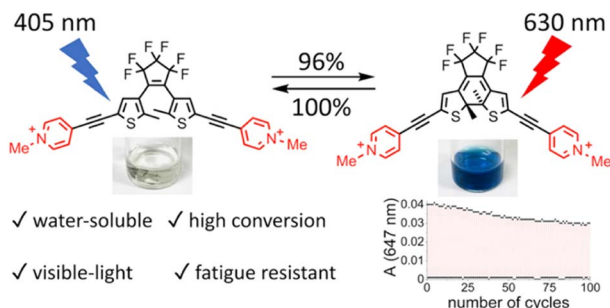
9114



### A host potassiophilicity strategy for unprecedentedly stable and safe K metal batteries

Zhibin Li, Liang Ma, Kai Han, Yingying Ji, Junpeng Xie, Likun Pan, Jinliang Li\* and Wenjie Mai\*

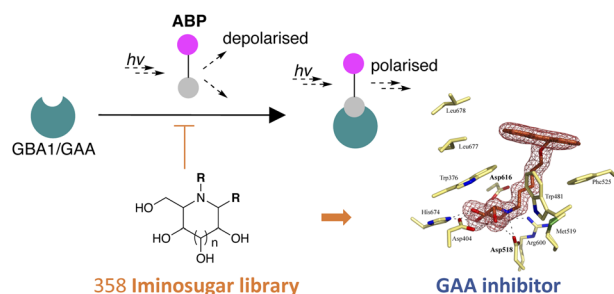
9123



### How do donor and acceptor substituents change the photophysical and photochemical behavior of dithienylethenes? The search for a water-soluble visible-light photoswitch

Sili Qiu, Andrew T. Frawley,\* Kathryn G. Leslie and Harry L. Anderson\*

9136



### Fluorescence polarisation activity-based protein profiling for the identification of deoxynojirimycin-type inhibitors selective for lysosomal retaining alpha- and beta-glucosidases

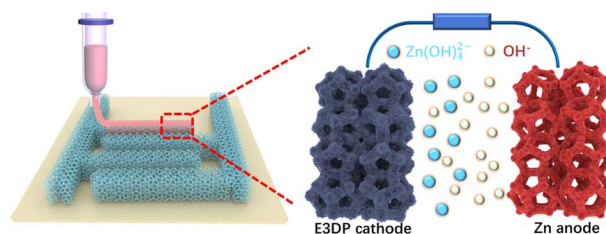
Daniël van der Gracht, Rhianna J. Rowland, Véronique Roig-Zamboni, Maria J. Ferraz, Max Louwerse, Paul P. Geurink, Johannes M. F. G. Aerts, Gerlind Sulzenbacher, Gideon J. Davies, Herman S. Overkleeft\* and Marta Artola\*



9145

### Achieving desirable charge transport by porous frame engineering for superior 3D printed rechargeable Ni–Zn alkaline batteries

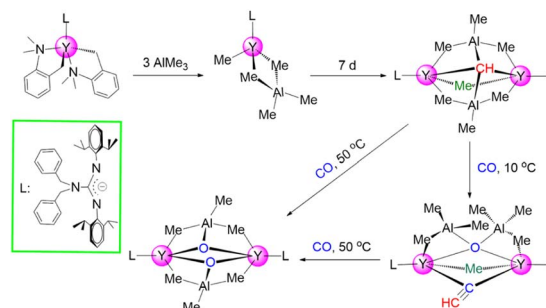
Wenyu Cao, Haojie Li, Hui Ma, Jintao Fan and Xiaocong Tian\*



9154

### A binuclear guanidinate yttrium carbyne complex: unique reactivity toward unsaturated C–N, C–O and C–S bonds

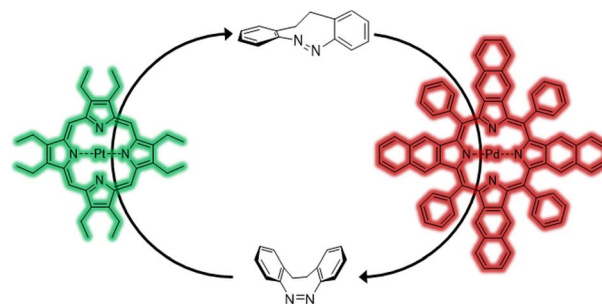
Wen Jiang, Feng Kong, Iker del Rosal, Meng Li, Kai Wang, Laurent Maron\* and Lixin Zhang\*



9161

### Triplet sensitization enables bidirectional isomerization of diazocine with 130 nm redshift in excitation wavelengths

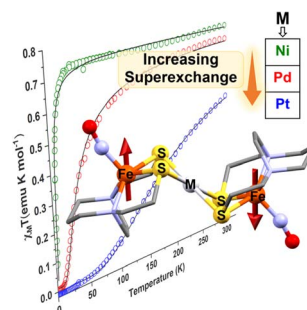
Jussi Isokuortti, Thomas Griebenow, Jan-Simon von Glasenapp, Tim Raeker, Mikhail A. Filatov, Timo Laaksonen, Rainer Herges\* and Nikita A. Durandin\*



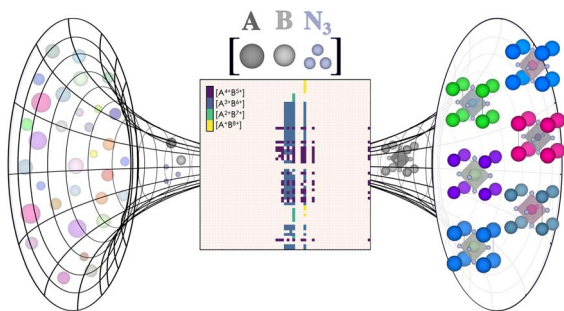
9167

### Magnetic coupling between Fe(NO) spin probe ligands through diamagnetic Ni<sup>II</sup>, Pd<sup>II</sup> and Pt<sup>II</sup> tetrathiolate bridges

Manuel Quiroz, Molly M. Lockart, Shan Xue, Dakota Jones, Yisong Guo, Brad S. Pierce, Kim R. Dunbar,\* Michael B. Hall\* and Marcetta Y. Darensbourg\*



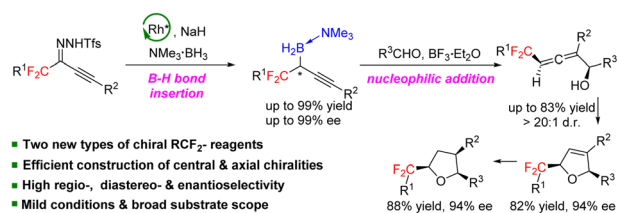
9175



### Accessible chemical space for metal nitride perovskites

Bastien F. Grosso, Daniel W. Davies, Bonan Zhu, Aron Walsh\* and David O. Scanlon\*

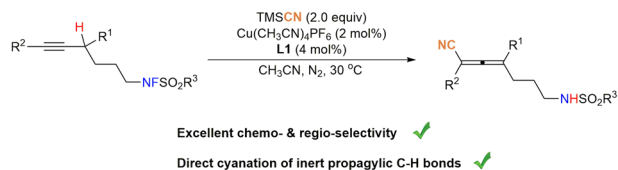
9186



### Chiral *gem*-difluoroalkyl reagents: *gem*-difluoroalkyl propargylic borons and *gem*-difluoroalkyl $\alpha$ -allenols

Hui-Na Zou, Meng-Lin Huang, Ming-Yao Huang, Yu-Xuan Su, Jing-Wei Zhang, Xin-Yu Zhang and Shou-Fei Zhu\*

9191

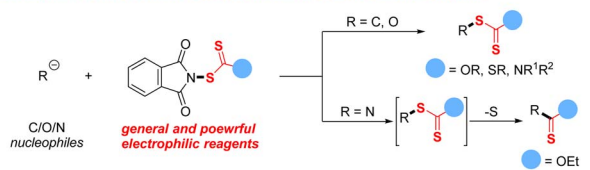


### Copper-catalyzed propargylic C–H functionalization for allene syntheses

Dongjie Zhang, Junjie Fan, Yaqi Shi, Yankai Huang, Chunling Fu, Xiaoyan Wu\* and Shengming Ma\*

9197

#### Electrophilic xanthylation via powerful phthalimide-carried transfer reagents



#### Highlighted features

- ◆ Broad reaction scope (C, O and desulfurization for N nucleophiles)
- ◆ Excellent tolerance
- ◆ Xanthylation, xanthamidation and thioxanthylation
- ◆ Late-stage electrophilic xanthylation

### Synthetic exploration of electrophilic xanthylation via powerful *N*-xanthylphthalimides

Shuo Wang, Liuqing Yang, Fangcan Liang, Yu Zhong, Xueru Liu, Qingling Wang\* and Dianhu Zhu\*

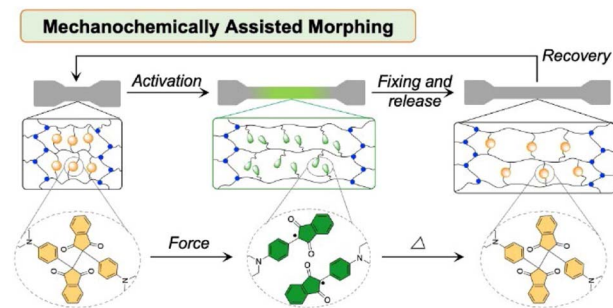




9207

### Mechanochemically assisted morphing of shape shifting polymers

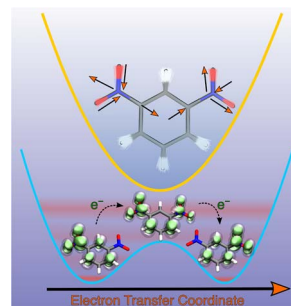
Rui Tang, Wenli Gao, Yulin Jia, Kai Wang, Barun Kumar Datta, Wei Zheng, Huan Zhang, Yuanze Xu, Yangju Lin\* and Wengui Weng\*



9213

### The Marcus dimension: identifying the nuclear coordinate for electron transfer from *ab initio* calculations

Adam Šrut, Benjamin J. Lear\* and Vera Krewald\*



9226

### Correction: 2-Mercaptomethyl-thiazolidines use conserved aromatic–S interactions to achieve broad-range inhibition of metallo- $\beta$ -lactamases

Maria-Agustina Rossi, Veronica Martinez, Philip Hinchliffe, Maria F. Mojica, Valerie Castillo, Diego M. Moreno, Ryan Smith, Brad Spellberg, George L. Drusano, Claudia Banchio, Robert A. Bonomo, James Spencer, Alejandro J. Vila\* and Graciela Mahler\*

9227

### Correction: A visible-light-driven molecular motor based on barbituric acid

Kim Kuntze, Daisy R. S. Pooler, Mariangela Di Donato, Michiel F. Hilbers, Pieter van der Meulen, Wybren Jan Buma, Arri Priimagi, Ben L. Feringa\* and Stefano Crespi\*

