### **Chemical Science**

#### rsc.li/chemical-science

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 2041-6539 CODEN CSHCBM 14(12) 3079-3388 (2023)



#### Cover

See Regina de Vivie-Riedle et al., pp. 3117-3131. Image reproduced by permission of Vera Hiendl from Chem. Sci., 2023, 14, 3117. Artwork created by Vera Hiendl/econversion.



#### Inside cover

See Shunxi Dong et al., pp. 3132-3139. Image reproduced by permission of Shiyu Wang from Chem. Sci., 2023, 14, 3132.

#### **REVIEW**

3091

#### Conductive hydrogels for tissue repair

Yongping Liang, Lipeng Qiao, Bowen Qiao and Baolin Guo\*

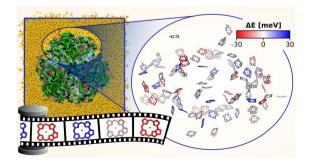


#### **EDGE ARTICLES**

3117

#### Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations

Sebastian Reiter, Ferdinand L. Kiss, Jürgen Hauer and Regina de Vivie-Riedle\*



#### **Editorial Staff**

**Executive Editor** 

May Copsey

**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

For pre-submission queries please contact May Copsey, Executive Editor.

E-mail 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 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

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

## **Chemical Science**

#### 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 Vy Dong, University of California, Irvine François Gabbaĭ, Texas A&M University Subi George, JNCASR Jinlong Gong, Tianjin University Stephen Goldup, University of Southampton 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

#### **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

R. Granam 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 Dalls

Elizabeth Gibson, Newcastle University Ryan Gilmour, WWU Münster 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

Jerôme Lacour, University of Geneva Ai-Lan Lee, Heriot-Watt University Daniele Leonori, University of Manchester 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 Mindiola, 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

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

Andrei Yudin, University of Toronto

Stuart Rowan, University of Chicago Richmond Sarpong, University of California, Berkelev

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 Mortin

David Spring, University of Cambridge Brian Stoltz, California Institute of Technology Brent Sumerlin, University of Florida Raghavan B. Sunoj, IIT Bombay Yogesh Surendranath, MIT Mizuki Tada, Nagoya University Ben Zhong Tang, The Hong Kong University of Science and Technology Zhiyong Tang, National Center for

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, Berkley
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

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



#### 3132

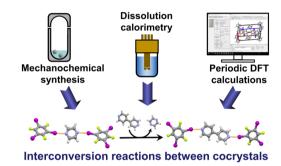
Regioselective C-H alkylation of anisoles with olefins by cationic imidazolin-2-iminato scandium(III) alkyl complexes

Shiyu Wang, Chenhao Zhu, Lichao Ning, Dawei Li, Xiaoming Feng and Shunxi Dong\*

#### 3140

Computational evaluation of halogen-bonded cocrystals enables prediction of their mechanochemical interconversion reactions

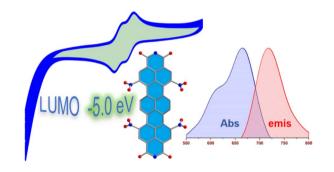
Lavanya Kumar, Katarina Leko, Vinko Nemec, Damian Trzybiński, Nikola Bregović, Dominik Cinčić and Mihails Arhangelskis\*



#### 3147

The deeper it goes, the brighter it glows: NIR emissive nitro-terrylene diimides with deep LUMOs

Kundan Singh Mehra, Shivangee Jha, Anila M. Menon, Deepak Chopra and Jeyaraman Sankar\*

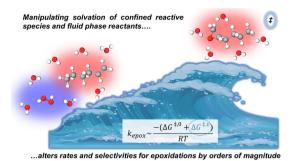


#### 3154

**Enantioselective direct Michael addition of** cyanohydrin ether derivatives to enones catalyzed by chiral bis(quanidino)iminophosphorane organosuperbase

Saikat Das, Azusa Kondoh\* and Masahiro Terada\*

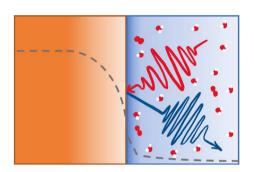
#### 3160



Engineering intraporous solvent environments: effects of aqueous-organic solvent mixtures on competition between zeolite-catalyzed epoxidation and  $\rm H_2O_2$  decomposition pathways

David S. Potts, Chris Torres, Ohsung Kwon and David W. Flaherty\*

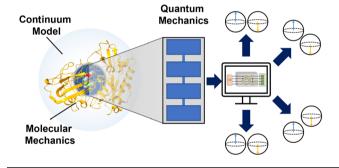
#### 3182



## Monitoring interfacial electric fields at a hematite electrode during water oxidation

Khezar H. Saeed, Dora-Alicia Garcia Osorio, Chao Li, Liam Banerji, Adrian M. Gardner and Alexander J. Cowan\*

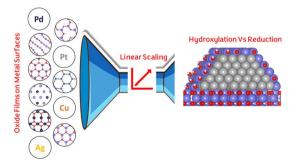
#### 3190



## Multiscale quantum algorithms for quantum chemistry

Huan Ma, Jie Liu, \* Honghui Shang, \* Yi Fan, Zhenyu Li and Jinlong Yang \*

#### 3206



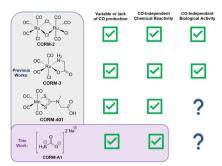
# Universal properties of metal-supported oxide films from linear scaling relationships: elucidation of mechanistic origins of strong metal-support interactions

Kaustubh J. Sawant, Zhenhua Zeng and Jeffrey P. Greeley\*

#### 3215

Reassessing CORM-A1: redox chemistry and idiosyncratic CO-releasing characteristics of the widely used carbon monoxide donor

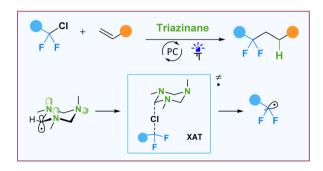
Nicola Bauer, Xiaoxiao Yang, Zhengnan Yuan and Binghe Wang\*



#### 3229

#### Aminals as powerful XAT-reagents: activation of fluorinated alkyl chlorides

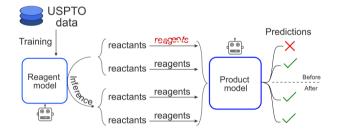
Vladislav S. Kostromitin, Artem O. Sorokin, Vitalij V. Levin and Alexander D. Dilman\*



#### 3235

#### Reagent prediction with a molecular transformer improves reaction data quality

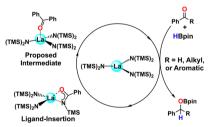
Mikhail Andronov,\* Varvara Voinarovska, Natalia Andronova, Michael Wand, Djork-Arné Clevert and Jürgen Schmidhuber



#### 3247

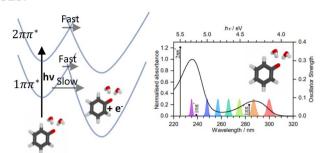
#### Mechanistic study of homoleptic trisamidolanthanide-catalyzed aldehyde and ketone hydroboration. Chemically non-innocent ligand participation

Jacob O. Rothbaum, Alessandro Motta,\* Yosi Kratish\* and Tobin J. Marks\*



- Proposed Intermediate & Deactivated Complexes Isolated
   Multinuclear NMR Stoichiometric & Solid-State Studies
   Experimental Evidence Favoring Ligand-Assisted Mechanism
   DFT Mechanistic Insight into Aldehyde & Ketone Hydroborati

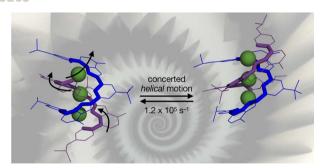
#### 3257



## Wavelength dependent mechanism of phenolate photooxidation in aqueous solution

Kate Robertson, William G. Fortune, Julia A. Davies, Anton N. Boichenko, Michael S. Scholz, Omri Tau, Anastasia V. Bochenkova and Helen H. Fielding\*

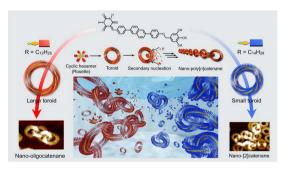
#### 3265



## Helical fluxionality: numerical frustration drives concerted low-barrier screw motions of a tricopper cluster

Heechan Kim, Juhwan Shin, Seyong Kim and Dongwhan Lee\*

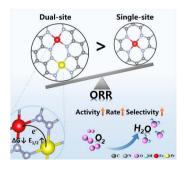
#### 3270



# Fine-tuning of the size of supramolecular nanotoroids suppresses the subsequent catenation of nano-[2]catenane

Hiroki Itabashi, Sougata Datta, Ryohei Tsukuda, Martin J. Hollamby and Shiki Yagai<sup>\*</sup>

#### 3277



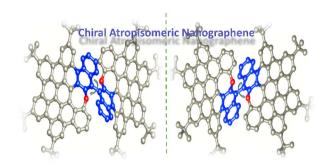
# Modulating the electronic structure of atomically dispersed Fe-Pt dual-site catalysts for efficient oxygen reduction reactions

Wei-Shen Song, Mei Wang, Xiao Zhan, Yan-Jie Wang, Dong-Xu Cao, Xian-Meng Song, Zi-Ang Nan, Li Zhang\* and Feng Ru Fan\*

#### 3286

#### BINOL-like atropisomeric chiral nanographene

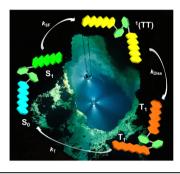
Shengtao Li, Ranran Li, Yi-Kang Zhang, Shutao Wang, Bin Ma, Bin Zhang and Peng An\*



#### 3293

#### Control of intramolecular singlet fission in a pentacene dimer by hydrostatic pressure

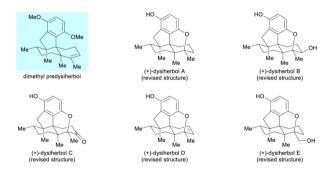
Tomokazu Kinoshita, Shunta Nakamura, Makoto Harada, Taku Hasobe\* and Gaku Fukuhara\*



#### 3302

#### Divergent total synthesis of the revised structures of marine anti-cancer meroterpenoids (+)-dysiherbols A-E

Chuanke Chong, Le Chang, Isabelle Grimm, Qunlong Zhang, Yang Kuang, Bingjian Wang, Jingyi Kang, Wenhui Liu, Julian Baars, Yuanqiang Guo, Hans-Günther Schmalz\* and Zhaoyong Lu\*



#### 3311

#### Degradable polyisoprene by radical ring-opening polymerization and application to polymer prodrug nanoparticles

Maëlle Lages, Théo Pesenti, Chen Zhu, Dao Le, Julie Mougin, Yohann Guillaneuf and Julien Nicolas\*



#### 3326

# Tailoring MR Emitter with Dynamic Bond Interactions Enhanced Rigidity by H-bond Dynamic Bond Interactions Enhanced Rigidity by H-bond William Parent Unique Assembly by N-B dative bond High Performance OLEDs

# Dynamic bond interactions fine-tune the properties of multiple resonance emitters towards highly efficient narrowband green OLEDs

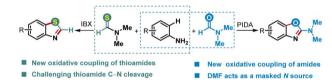
Yang Zou, Mingxin Yu, Jingsheng Miao,\* Taian Huang, Shuokun Liao, Xiaosong Cao and Chuluo Yang

3332

# Combining photoredox catalysis and hydrogen atom transfer for dearomative functionalization of electron rich heteroarenes

Peng Ji, Xiang Meng, Jing Chen, Feng Gao, Hang Xu and Wei Wang\*

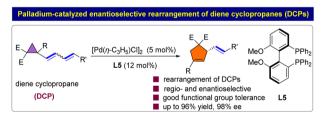
3338



## Hypervalent iodine-promoted twofold oxidative coupling of amines with amides and thioamides: chemoselective pathway to oxazoles and thiazoles

Jiang Nan,\* Xin Ren, Qiang Yan, Shilei Liu, Jing Wang, Yangmin Ma and Michal Szostak\*

3346



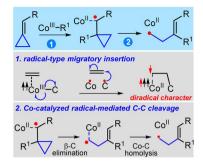
## Palladium-catalyzed enantioselective rearrangement of dienyl cyclopropanes

Qi Xu, Chuan-Jun Lu, Chang-Qiu Guo, Jia Feng and Ren-Rong Liu\*

#### 3352

#### Cobalt-catalyzed radical-mediated carbon-carbon scission via a radical-type migratory insertion

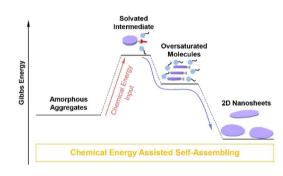
Jian-Biao Liu, \* Xiao-Jun Liu, João C. A. Oliveira, De-Zhan Chen and Lutz Ackermann\*



#### 3363

#### Chemical energy assisted self-assembling of a porphyrin-substituted benzoic acid in complex environments

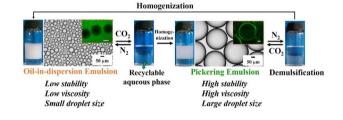
Bingxu Ma, Bowen Pang, Wang Zeng,\* Huimin Fu, Yi Jiang, Shenglin Yao, Yida Yang, Kaisheng Zhu and Wei Zhang\*



#### 3370

#### CO<sub>2</sub>-switchable emulsions with controllable size and viscosity

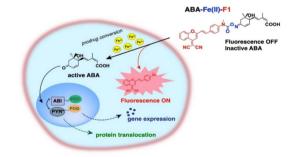
Jianzhong Jiang,\* Huaixin Li and Yao Gu



#### 3377

#### A theranostic abscisic acid-based molecular glue

Jing Chen, Huong T. X. Nguyen, Ming Yang, Fangxun Zeng, Hang Xu, Fu-Sen Liang\* and Wei Wang\*



#### **CORRECTIONS**

3385

Correction: Isolation of C1 through C4 derivatives from CO using heteroleptic uranium(III) metallocene aryloxide complexes

Robert J. Ward, Iker del Rosal, Steven P. Kelley, Laurent Maron\* and Justin R. Walensky\*

3386

Correction: Multi-stimuli programmable FRET based RGB absorbing antennae towards ratiometric temperature, pH and multiple metal ion sensing

Kavita Rani and Sanchita Sengupta\*