

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(46) 13267–13588 (2023)



### Cover

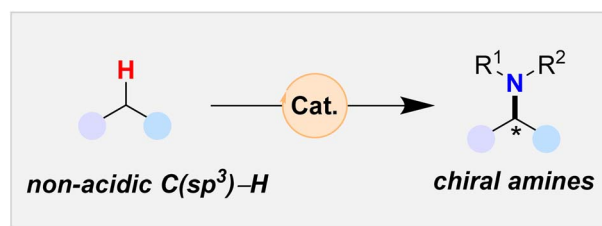
See Oleg V. Larionov *et al.*, pp. 13384–13391. Image reproduced by permission of Oleg V. Larionov from *Chem. Sci.*, 2023, 14, 13384.

## PERSPECTIVES

13278

### Recent developments for intermolecular enantioselective amination of non-acidic C(sp<sup>3</sup>)-H bonds

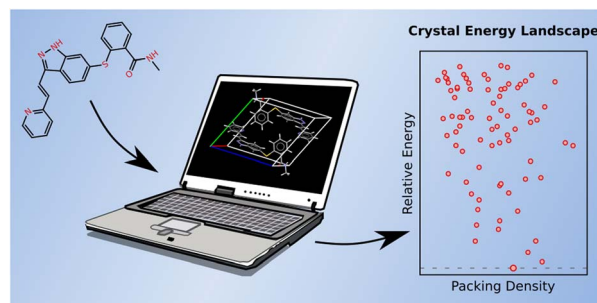
Heng-Hui Li, Xuemeng Chen and Søren Kramer\*



13290

### Frontiers of molecular crystal structure prediction for pharmaceuticals and functional organic materials

Gregory J. O. Beran



# 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

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

D. Adams, University of Glasgow  
A. Ajayaghosh, NIIST  
R. Amaro, UC San Diego  
A. Anastasaki, ETH Zürich  
U.-P. Apfel, Ruhr-University Bochum  
K. Asmis, Leipzig University  
X. Bao, DICP-CAS  
Z. Bao, Stanford University  
D. N. Beratan, Duke University  
G. Bernardes, University of Cambridge  
F. Biedermann, KIT  
D. Blackmond, Scripps Research Institute  
E. Blasco, Heidelberg University  
J. Bode, ETH Zurich  
J. S. Brodbelt, UT Austin  
C. Chang, UC Berkeley  
C.-M. Che, University of Hong Kong  
J. Chen, Nankai University  
M. Cohen, OHSU  
C. Coley, MIT  
J. Cornella, MPIC  
L. Cronin, University of Glasgow  
J. Crowley, University of Otago  
C. C. Cummins, MIT  
V. Däschlein-Gessner, Ruhr University Bochum  
M. Delbianco, MPICI  
J. Dempsey, UNC Chapel Hill  
W. Dichtel, Northwestern University  
K. Domen, University of Tokyo  
H. Duan, Tsinghua University  
X. Feng, TU Dresden  
B. Feringa, University of Groningen  
J. Figueroa, UC San Diego  
N. Frank, University of Nevada  
M. Freitag, Newcastle University  
S. Gao, Peking University  
J. Gassensmith, UT Dallas  
G. Gasser, PSL University  
E. Gibson, Newcastle University  
R. Gilliard, Jr., MIT  
F. Glorius, WWU Münster  
L. González, University of Vienna  
D. Graham, University of Strathclyde  
V. Grassian, UC San Diego  
A. Grimaud, Collège de France/CNRS  
T. Gulder, Leipzig University  
W. Gutkunst, Georgia Tech  
C. Hackenberger, FMP Berlin  
I. Hamachi, Kyoto University  
G. Han, Brandeis University  
B. Han, CAS

M. Hariharan, IISER-TVM  
C. Haynes, University of Minnesota  
J. Heemstra, WUSTL  
T. Heine, DTU  
P. Holland, Yale University  
K. E. Jelfs, Imperial College London  
X. Jiang, Aramco  
Y. Jung, SNU  
S. Kath-Schorr, University of Cologne  
T. Kato, University of Tokyo  
C. Kelly, Janseen Research/J&J  
R. Klausen, Johns Hopkins University  
Y. Krishnan, University of Chicago  
M. Kuimova, Imperial College London  
K. Lancaster, Cornell University  
A.-L. Lee, Heriot-Watt University  
D. Leonori, University of Manchester  
X. Li, University of Washington  
Y. Li, Jilin University  
M. H. Lim, KAIST  
J. Lloret-Fillol, ICIQ  
B. Lotsch, Max Planck Institute  
X. W. Lou, NTU  
K. Maeda, Tokyo Tech  
S. Maeda, Hokkaido University  
D. Maiti, IIT Bombay  
L. Malins, ANU  
S. Mandal, IISER Kolkata  
T. Martinez, Stanford University  
C. Martínez-Huitle, UFRN  
E. Matson, Rochester University  
J. L. Medina-Franco, UNAM  
V. Moliner, INAM, Jaume I University  
W. Nam, Ewha Womans University  
T. Noël, University of Amsterdam  
A. Obermeyer, Columbia University  
M. Oestreich, TU Berlin  
D. O'Hagan, University of St Andrews  
T. Ooi, Nagoya University  
R. O'Reilly, University of Birmingham  
S. Ott, Uppsala University  
H. Ottosson, Uppsala University  
Z. Ouyang, Tsinghua University  
X. Pan, DICP-CAS  
S. Patil, SSCU-IISC  
E. Pentzer, Texas A&M University  
S. Peter, JNCASR  
W. Piers, University of Calgary  
N. Plumeré, Ruhr-University Bochum  
S. Qiao, University of Adelaide  
V. Rai, IISER Bhopal

S. Rasmussen, North Dakota State University  
J. Read de Alaniz, UC Santa Barbara  
E. Reisner, University of Cambridge  
A. Rentmeister, WWU Münster  
J. Rinehart, UC San Diego  
A. Roitberg, University of Florida  
H. Sardon, UPV-EHU  
R. Sarpong, UC Berkeley  
G. Schultz, Northwestern University  
D. Schultz, Merck  
D. Seferos, University of Toronto  
R. Sessoli, University of Florence  
H. Shafaat, UCLA  
T. Snaddon, Indiana University  
M. Solà, University of Girona  
G. Soler-Illia, UNSAM  
D. Spring, University of Cambridge  
B. Sumerlin, University of Florida  
R. B. Sunoj, IIT Bombay  
Y. Surendranath, MIT  
M. Tada, Nagoya University  
T. Tahara, RIKEN  
Z. Tang, NCSNT  
S. Teichert, DESY  
C. Thomas, Ohio State University  
H. Tian, ECUST  
Z.-Q. Tian, Xiamen University  
A. Tkatchenko, University of Luxembourg  
H. Tran, University of Toronto  
T. Uemura, University of Tokyo  
C. Vanderwal, UC Irvine  
L. Venkataraman, Columbia University  
G. Vilé, Politecnico di Milano  
A. Wakamiya, Kyoto University  
L.-S. Wang, Brown University  
C. Wang, Peking University  
E. Weerapana, Boston College  
J. Weinstein, University of Sheffield  
T. Welton, Imperial College London  
A. Wendlandt, MIT  
C. Williams, University of Oxford  
V. Yam, University of Hong Kong  
N. Yanai, Kyushu University  
S. Q. Yao, National University of Singapore  
A. Zharbin, UFPR  
L. Zhang, ECNU  
T. Zhang, TIPCC-CAS  
J. Zhang, University of Cambridge  
Z.-J. Zhao, Tianjin University  
B. Zhong Tang, CUHK-Shenzhen  
Q.-L. Zhou, Nankai University

## Editorial Staff

### Executive Editor

May Copsy

### Deputy Editor

Samantha Apps

### Senior Editor

James Moore

### Scientific Editors

Ellis Crawford, 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)

## 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/publish 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



## PERSPECTIVES

13313

## Two-dimensional mesoporous metals: a new era for designing functional electrocatalysts

Hao Lv and Ben Liu\*

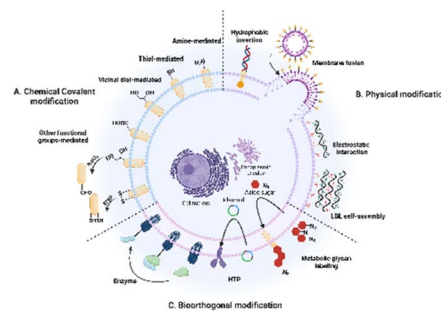


## REVIEWS

13325

## Advancing cell surface modification in mammalian cells with synthetic molecules

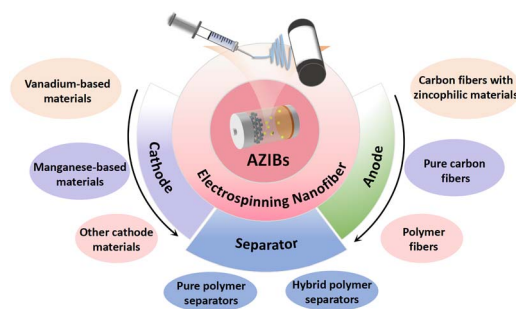
He Yang, Lihua Yao, Yichen Wang, Gaojian Chen\* and Hong Chen\*



13346

## Recent advances in electrospinning nanofiber materials for aqueous zinc ion batteries

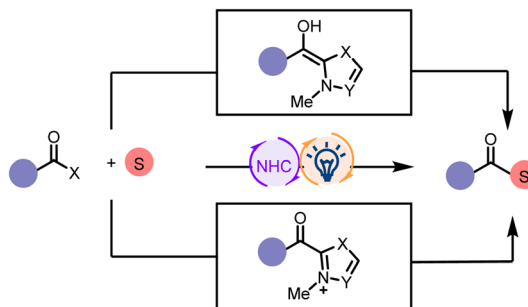
Sinian Yang, Shunshun Zhao and Shimou Chen\*



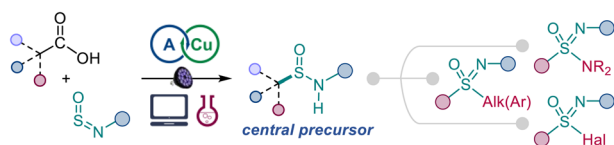
13367

## Recent advances in combining photo- and N-heterocyclic carbene catalysis

Xiaochen Wang, Senhui Wu, Rongxin Yang, Hongjian Song, Yuxiu Liu and Qingmin Wang\*



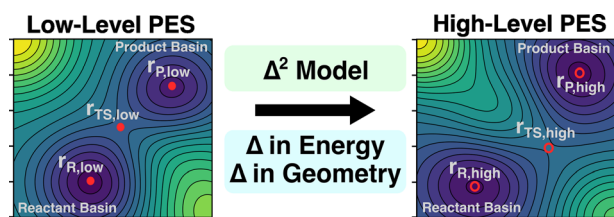
13384



### Kinetically-driven reactivity of sulfinylamines enables direct conversion of carboxylic acids to sulfinamides

Hang T. Dang, Arka Porey, Sachchida Nand, Ramon Trevino, Patrick Manning-Lorino, William B. Hughes, Seth O. Fremin, William T. Thompson, Shree Krishna Dhakal, Hadi D. Arman and Oleg V. Larionov\*

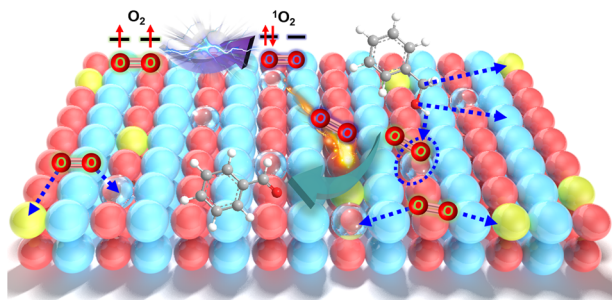
13392



### $\Delta^2$ machine learning for reaction property prediction

Qiyuan Zhao, Dylan M. Anstine, Olexandr Isayev\* and Brett M. Savoie\*

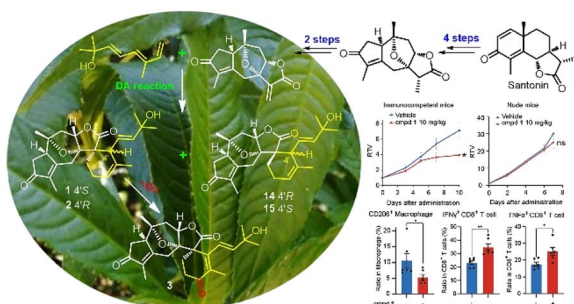
13402



### Spontaneous generation of singlet oxygen on microemulsion-derived manganese oxides with rich oxygen vacancies for efficient aerobic oxidation

Jun Tang, Junbao Chen, Zhanyu Zhang, Qincheng Ma, Xiaolong Hu, Peng Li, Zhiqiang Liu, Peixin Cui, Chao Wan,\* Qingping Ke,\* Lei Fu, Jeonghun Kim, Takashi Hamada, Yunqing Kang\* and Yusuke Yamauchi\*

13410



### Unprecedented sesterterpenoids, orientanoids A–C: discovery, bioinspired total synthesis and antitumor immunity

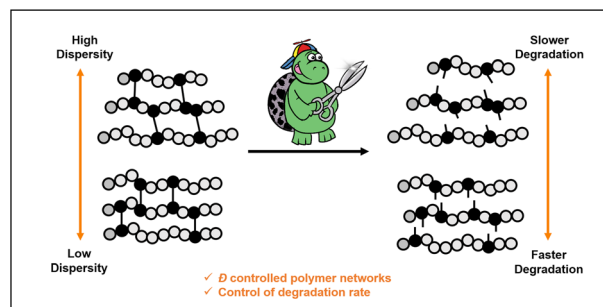
Cheng-Yu Zheng, Jin-Xin Zhao, Chang-Hao Yuan, Xia Peng, Meiyu Geng, Jing Ai,\* Yao-Yue Fan\* and Jian-Min Yue\*



13419

### Controlling primary chain dispersity in network polymers: elucidating the effect of dispersity on degradation

Takanori Shimizu, Richard Whitfield,\* Glen R. Jones, Ibrahim O. Raji, Dominik Konkolewicz, Nghia P. Truong and Athina Anastasaki\*



13429

### Regioselective *ortho* halogenation of *N*-aryl amides and ureas *via* oxidative halodeboronation: harnessing boron reactivity for efficient C–halogen bond installation

Ganesh H. Shinde, Ganesh S. Ghotekar, Francoise M. Amombo Noa, Lars Öhrström, Per-Ola Norrby and Henrik Sundén\*

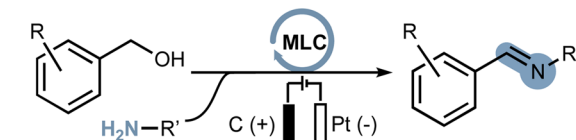


13437

### Merging electrocatalytic alcohol oxidation with C–N bond formation by electrifying metal–ligand cooperative catalysts

Sitthichok Kasemthaveechok, Patrice Gérardo and Niklas von Wolff\*

First molecular electrocatalytic C–N bond formation from alcohols



No amine oxidation  
low reaction potential  
high TON > 60  
> 30 examples

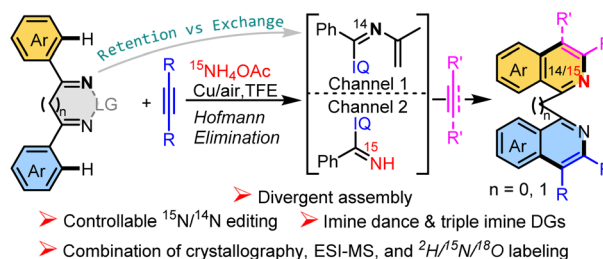
Electrification of MLC-catalysts



13446

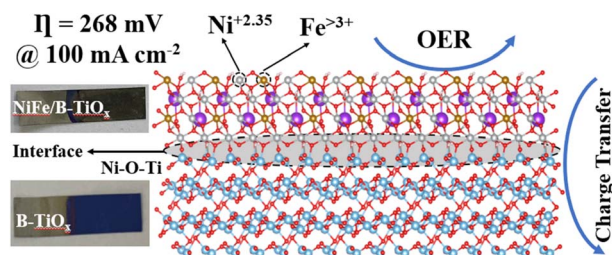
### Mechanistic insights into an $\text{NH}_4\text{OAc}$ -promoted imine dance in Rh-catalysed multicomponent double C–H annulations through an N-retention/exchange dual channel

Shiqing Li,\* Shihai Lv, Yanyan Yang, Peiyan Zhu, Dongbing Zhao\* and Ming-Hua Zeng\*





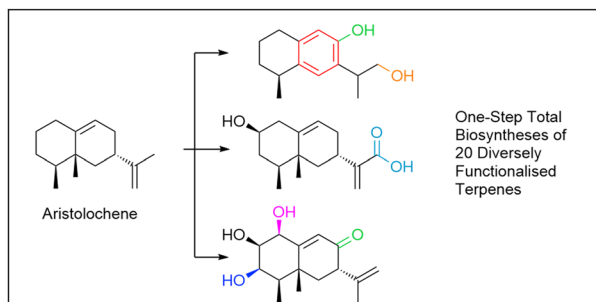
13453



### Defective blue titanium oxide induces high valence of NiFe-(oxy)hydroxides over heterogeneous interfaces towards high OER catalytic activity

Tingxi Zhou, Yifei Yang, Yike Jing, Yuling Hu, Fei Yang, Wei Sun\* and LeiLei He\*

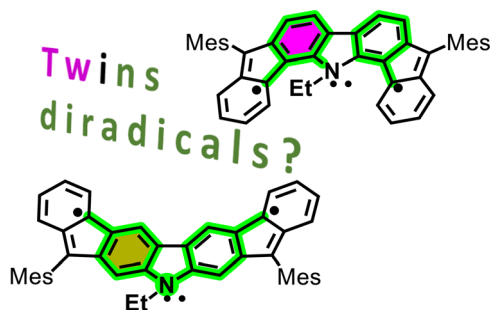
13463



### Rapid discovery of terpene tailoring enzymes for total biosynthesis

Yunlong Sun, Jennifer Gerke, Kevin Becker, Eric Kuhnert, Bart Verwaaijen, Daniel Wibberg, Jörn Kalinowski, Marc Stadler and Russell J. Cox\*

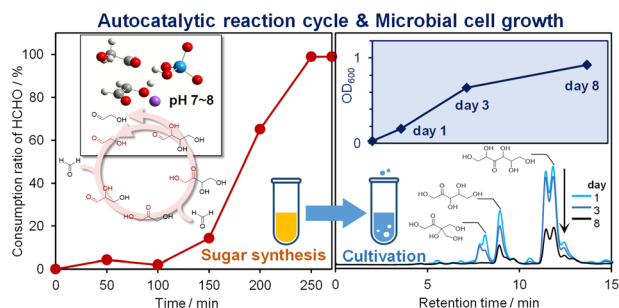
13468



### Isomerism tunes the diradical character of difluorenylpyrroles at constant Hückel-level anti-aromaticity

Ryotaro Moriyasu, Sergio Moles Quintero, Carlos J. Gómez-García, Kazumasa Suzuki, Chitoshi Kitamura, Michihisa Murata, Mercedes Alonso, Juan Casado\* and Shin-ichiro Kato\*

13475



### Construction of an autocatalytic reaction cycle in neutral medium for synthesis of life-sustaining sugars

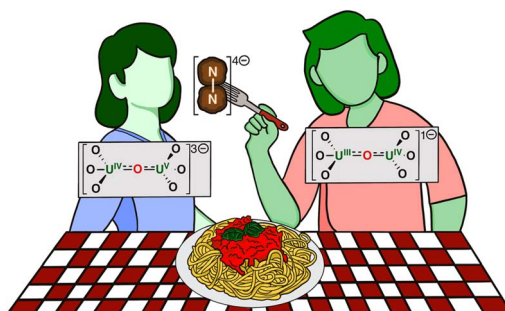
Hiro Tabata, Genta Chikatani, Hiroaki Nishijima, Takashi Harada, Rika Miyake, Souichiro Kato, Kensuke Igarashi, Yoshiharu Mukouyama, Soichi Shirai, Minoru Waki, Yoko Hase\* and Shuji Nakanishi\*



13485

### Dinitrogen cleavage by a dinuclear uranium(III) complex

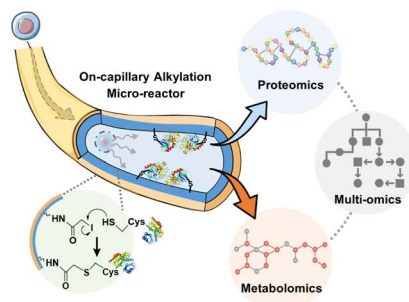
Nadir Jori, Megan Keener, Thayalan Rajeshkumar, Rosario Scopelliti, Laurent Maron\* and Marinella Mazzanti\*



13495

### On-capillary alkylation micro-reactor: a facile strategy for proteo-metabolome profiling in the same single cells

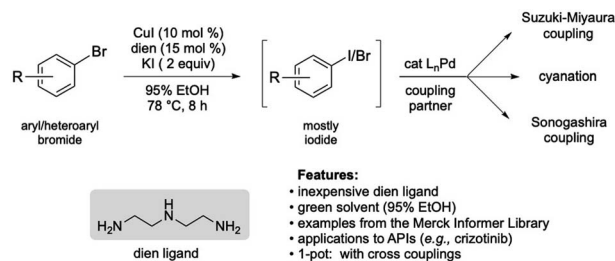
Yingyun He, Huiming Yuan,\* Yu Liang, Xinxin Liu, Xiaozhe Zhang, Yahui Ji, Baofeng Zhao, Kaiguang Yang, Jue Zhang, Shen Zhang, Yukui Zhang and Lihua Zhang\*



13503

### Challenging cross couplings, in water, aided by *in situ* iodination of (hetero)aromatic bromides

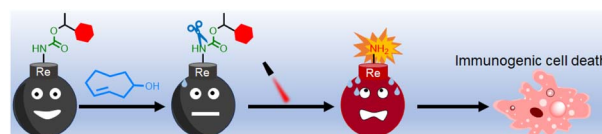
Rohan M. Thomas, David B. Obbard and Bruce H. Lipshutz\*



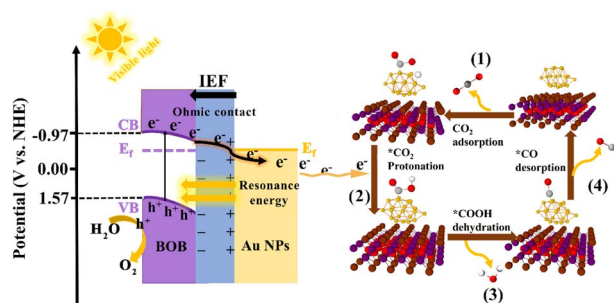
13508

### Bioorthogonal dissociative rhenium(I) photosensitisers for controlled immunogenic cell death induction

Guang-Xi Xu, Lawrence Cho-Cheung Lee, Peter Kam-Keung Leung, Eunice Chiu-Lam Mak, Justin Shum, Kenneth Yin Zhang, Qiang Zhao and Kenneth Kam-Wing Lo\*



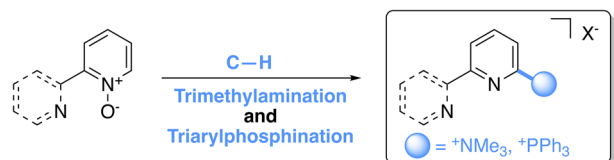
13518



### Synergistic coupling of interface ohmic contact and LSPR effects over Au/Bi<sub>24</sub>O<sub>31</sub>Br<sub>10</sub> nanosheets for visible-light-driven photocatalytic CO<sub>2</sub> reduction to CO

Jie Liu, Yu Xie,\* Yiqiao Wang, Kai Yang, Shuping Su, Yun Ling and Pinghua Chen

13530

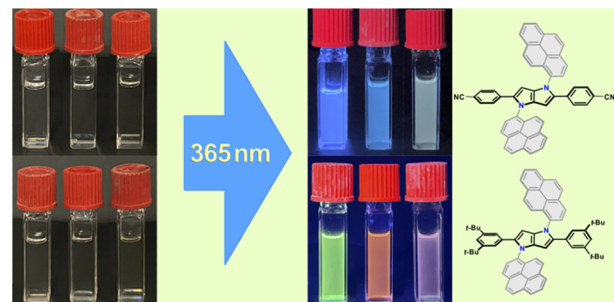


- One Pot
- Modular Synthesis
- Scalable (up to 5 g scale)
- Electrochemistry
- Metal Coordination
- Physical Properties

### Modular preparation of cationic bipyridines and azaarenes via C–H activation

Ryan P. King and Jenny Y. Yang\*

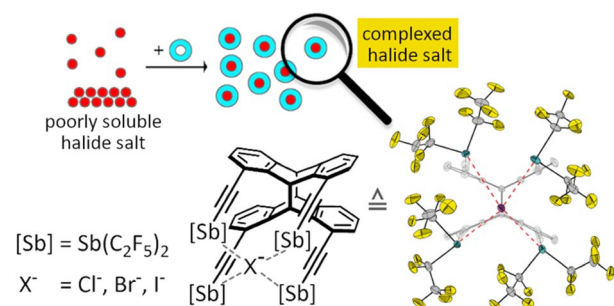
13537



### The magic of biaryl linkers: the electronic coupling through them defines the propensity for excited-state symmetry breaking in quadrupolar acceptor–donor–acceptor fluorophores

John A. Clark, Damian Kusy, Olena Vakuliuk, Maciej Krzeszewski, Krzysztof J. Kochanowski, Beata Koszarna, Omar O'Mari, Denis Jacquemin,\* Daniel T. Gryko\* and Valentine I. Vullev\*

13551



### Poly-pnictogen bonding: trapping halide ions by a tetradentate antimony(III) Lewis acid

J. Louis Beckmann, Jonas Krieft, Yury V. Vishnevskiy, Beate Neumann, Hans-Georg Stammer and Norbert W. Mitzel\*

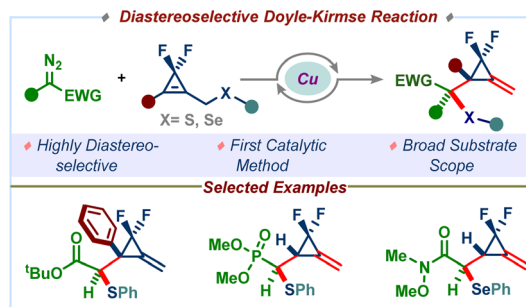




13560

### A highly diastereoselective strain-release Doyle–Kirmse reaction: access to functionalized difluoro(methylene)cyclopropanes

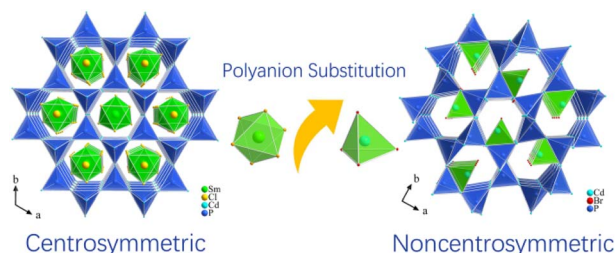
Suparnak Midya and Durga Prasad Hari\*



13568

### The first polyanion-substitution-driven centrosymmetric-to-noncentrosymmetric structural transformation realizing an excellent nonlinear optical supramolecule [Cd<sub>4</sub>P<sub>2</sub>][CdBr<sub>4</sub>]

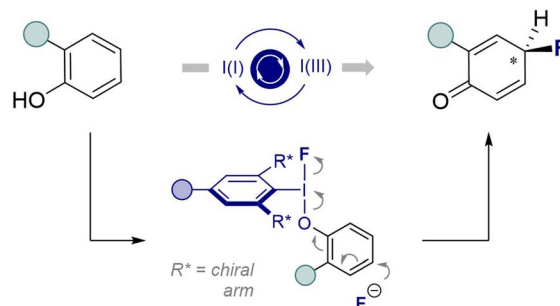
Zhi-Xin Qiu, Zhe-Xiong Zheng, Xiao-Ming Jiang, Bin-Wen Liu\* and Guo-Cong Guo\*



13574

### *para*-Selective dearomatization of phenols by I(I)/I(III) catalysis-based fluorination

Timo Stünkel, Kathrin Siebold, Daichi Okumatsu, Kazuki Murata, Louise Ruyet, Constantin G. Daniliuc and Ryan Gilmour\*



13581

### *Trans*-cyclosulfamidate mannose-configured cyclitol allows isoform-dependent inhibition of GH47 $\alpha$ -D-mannosidases through a bump–hole strategy

Alexandra Males, Ken Kok, Alba Nin-Hill, Nicky de Koster, Sija van den Beukel, Thomas J. M. Beenakker, Gijsbert A. van der Marel, Jeroen D. C. Codée, Johannes M. F. G. Aerts, Herman S. Overkleef, Carme Rovira,\* Gideon J. Davies\* and Marta Artola\*

