

IN THIS ISSUE

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



Cover

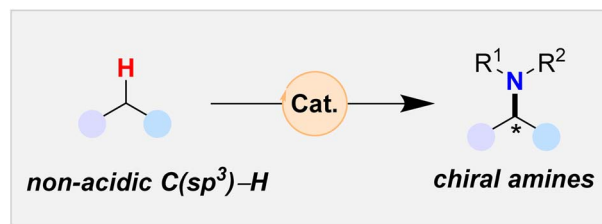
See Oleg V. Larionov *et al.*, pp. 13384–13391. Image reproduced by permission of Oleg V. Larionov from *Chem. Sci.*, 2023, 14, 13384.

PERSPECTIVES

13278

Recent developments for intermolecular enantioselective amination of non-acidic C(sp³)-H bonds

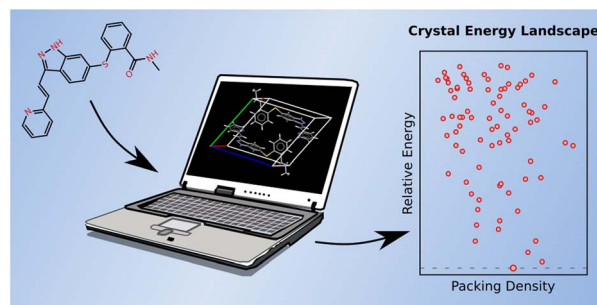
Heng-Hui Li, Xuemeng Chen and Søren Kramer*



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. Gutekunst, 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. Zarkin, 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

For pre-submission queries please contact May Copsy, 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

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/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

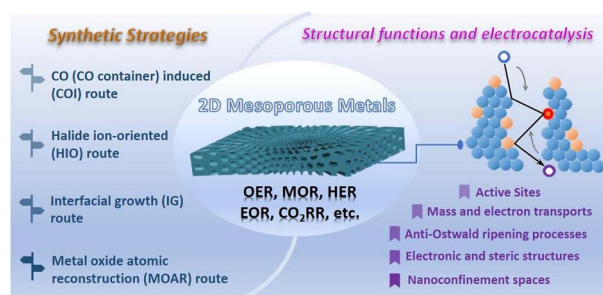


PERSPECTIVES

13313

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

Hao Lv and Ben Liu*

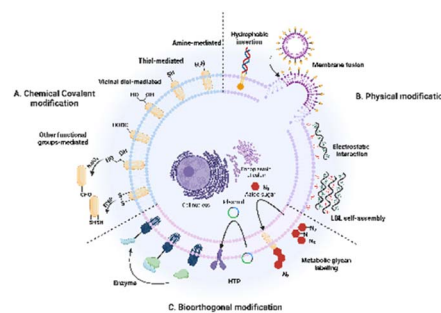


REVIEWS

13325

Advancing cell surface modification in mammalian cells with synthetic molecules

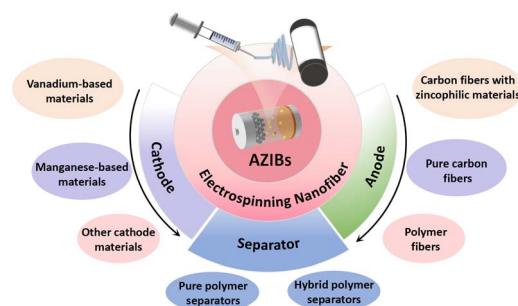
He Yang, Lihua Yao, Yichen Wang, Gaojian Chen* and Hong Chen*



13346

Recent advances in electrospinning nanofiber materials for aqueous zinc ion batteries

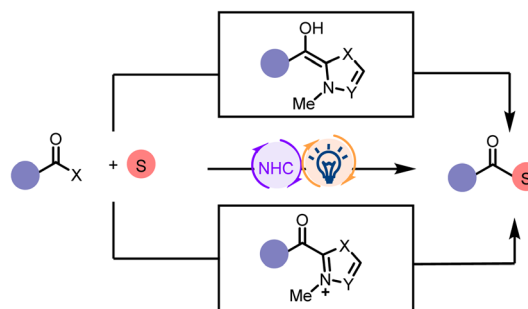
Sinian Yang, Shunshun Zhao and Shimou Chen*



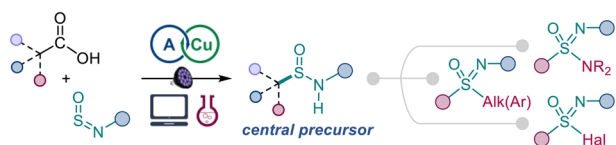
13367

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

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



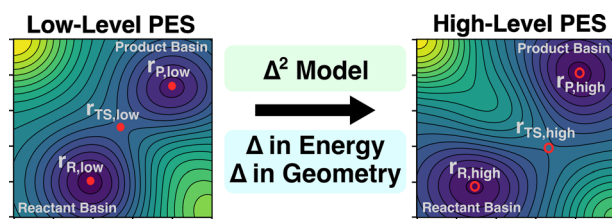
13384



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*

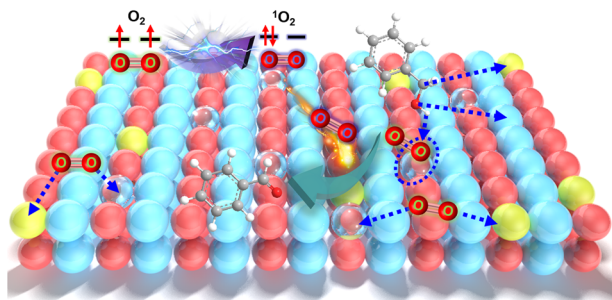
13392



Δ^2 machine learning for reaction property prediction

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

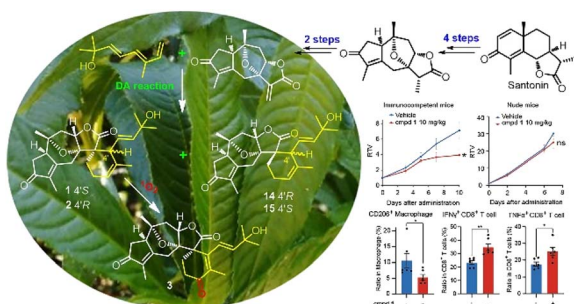
13402



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

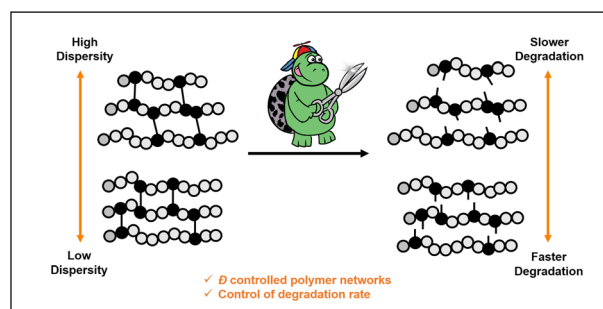
Cheng-Yu Zheng, Jin-Xin Zhao, Chang-Hao Yuan, Xia Peng, Meiyu Geng, Jing Ai,* Yao-Yue Fan* and Jian-Min Yue*



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*

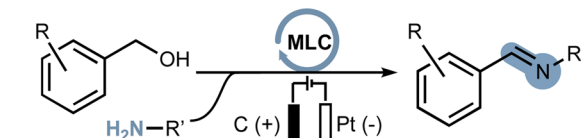


13437

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

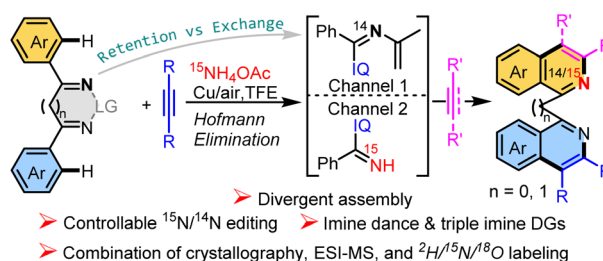
Electrification of MLC-catalysts



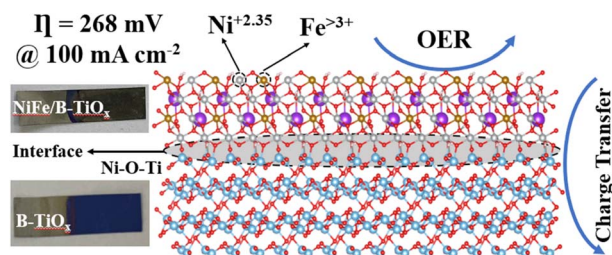
13446

Mechanistic insights into an NH_4OAc -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*



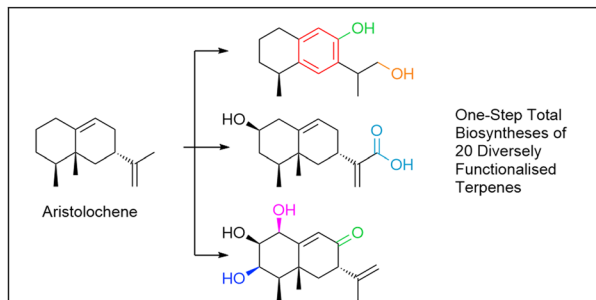
13453



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*

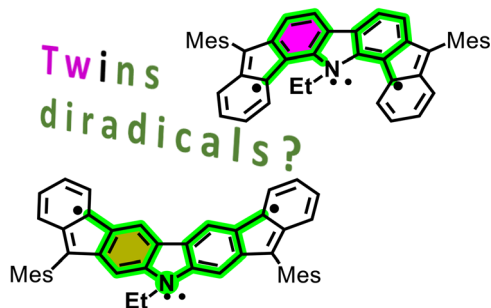
13463



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*

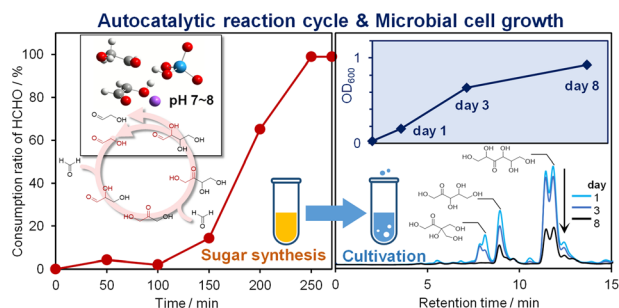
13468



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

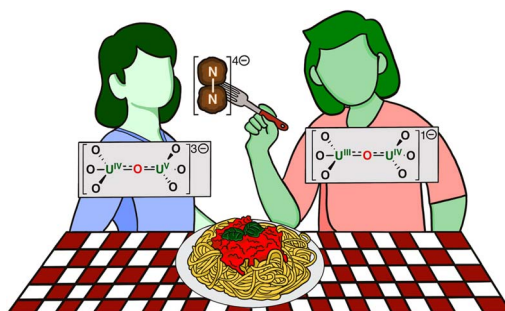
Hiro Tabata, Genta Chikatani, Hiroaki Nishijima, Takashi Harada, Rika Miyake, Souichiro Kato, Kensuke Igarashi, Yoshiharu Mukouyama, Soichi Shirai, Minoru Waki, Yoko Hase* and Shuji Nakanishi*



13485

Dinitrogen cleavage by a dinuclear uranium(III) complex

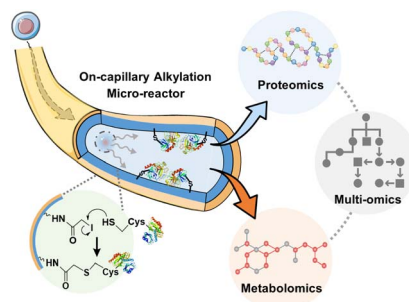
Nadir Jori, Megan Keener, Thayalan Rajeshkumar, Rosario Scopelliti, Laurent Maron* and Marinella Mazzanti*



13495

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

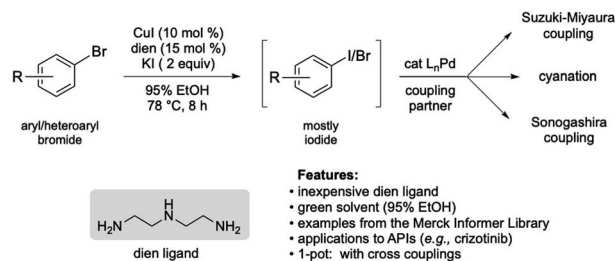
Yingyun He, Huiming Yuan,* Yu Liang, Xinxin Liu, Xiaozhe Zhang, Yahui Ji, Baofeng Zhao, Kaiguang Yang, Jue Zhang, Shen Zhang, Yukui Zhang and Lihua Zhang*



13503

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

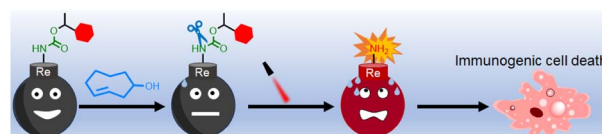
Rohan M. Thomas, David B. Obbard and Bruce H. Lipshutz*



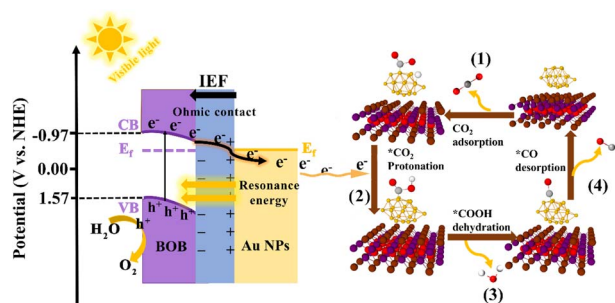
13508

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*



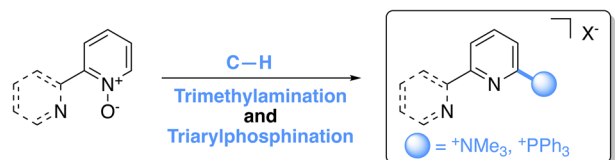
13518



Synergistic coupling of interface ohmic contact and LSPR effects over Au/Bi₂₄O₃₁Br₁₀ nanosheets for visible-light-driven photocatalytic CO₂ reduction to CO

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

13530

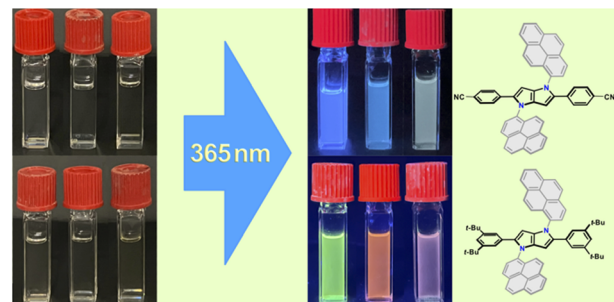


- One Pot
- Modular Synthesis
- Scalable (up to 5 g scale)
- Electrochemistry
- Metal Coordination
- Physical Properties

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

Ryan P. King and Jenny Y. Yang*

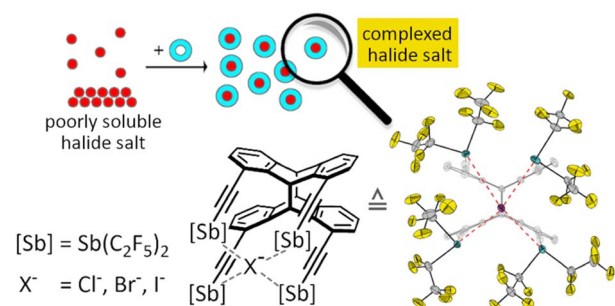
13537



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

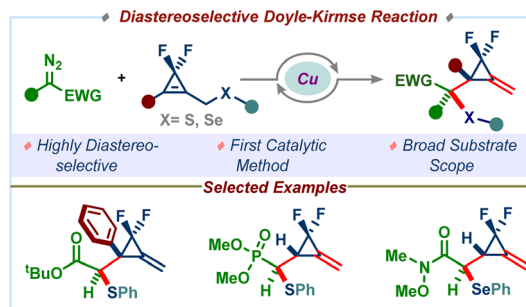
J. Louis Beckmann, Jonas Krieft, Yury V. Vishnevskiy, Beate Neumann, Hans-Georg Stammer and Norbert W. Mitzel*



13560

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

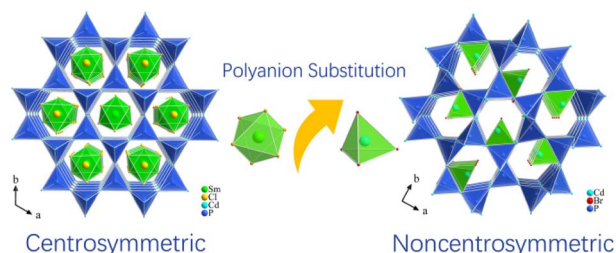
Suparnak Midya and Durga Prasad Hari*



13568

The first polyanion-substitution-driven centrosymmetric-to-noncentrosymmetric structural transformation realizing an excellent nonlinear optical supramolecule [Cd₄P₂][CdBr₄]

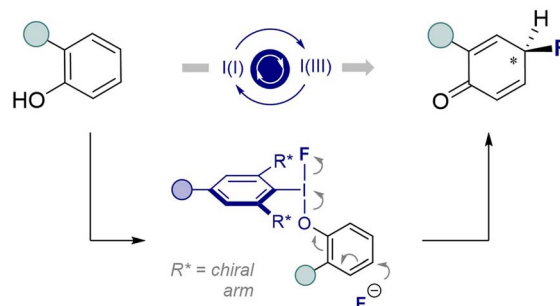
Zhi-Xin Qiu, Zhe-Xiong Zheng, Xiao-Ming Jiang, Bin-Wen Liu* and Guo-Cong Guo*



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 α -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*

