

IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(44) 12389–12800 (2023)



Cover
See Felipe García, Pablo García-Álvarez *et al.*, pp. 12477–12483. Image reproduced by permission of Clara Becedoniz Plasencia from *Chem. Sci.*, 2023, **14**, 12477.



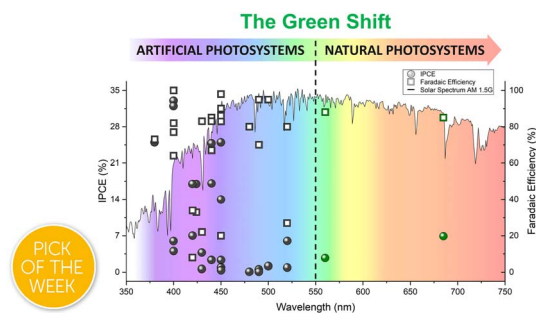
Inside cover
See Andrea Sartorel, Marcella Bonchio *et al.*, pp. 12402–12429. Image reproduced by permission of Marcella Bonchio from *Chem. Sci.*, 2023, **14**, 12402. Robin N. Dürr is thankfully acknowledged for designing and creating the cover artwork.

PERSPECTIVES

12402

A breath of sunshine: oxygenic photosynthesis by functional molecular architectures

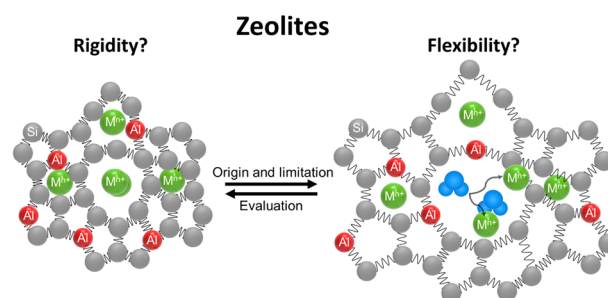
Thomas Gobbato, Giulia Alice Volpato, Andrea Sartorel* and Marcella Bonchio*



12430

Flexibility in zeolites: origin, limits, and evaluation

Sajjad Ghojavand, Eddy Dib and Svetlana Mintova*



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

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. Schutz, 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, TIPC-CAS
J. Zhang, University of Cambridge
Z.-J. Zhao, Tianjin University
B. Zhong Tang, CUHK-Shenzhen
Q.-L. Zhou, Nankai University

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

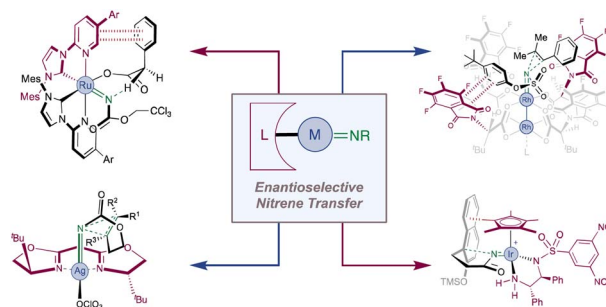


REVIEW

12447

Catalytic, asymmetric carbon–nitrogen bond formation using metal nitrenoids: from metal–ligand complexes *via* metalloporphyrins to enzymes

Alexander Fanourakis and Robert J. Phipps*

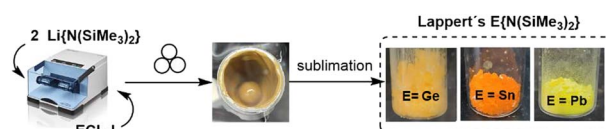


EDGE ARTICLES

12477

Fast and scalable solvent-free access to Lappert's heavier tetrylenes $E\{N(SiMe_3)_2\}_2$ ($E = Ge, Sn, Pb$) and $ECl\{N(SiMe_3)_2\}$ ($E = Ge, Sn$)

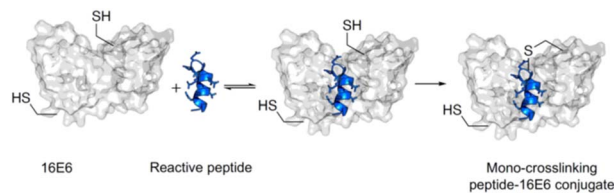
Javier A. Cabeza, Javier F. Reynes, Felipe García,* Pablo García-Álvarez* and Rubén García-Soriano



12484

Discovery of reactive peptide inhibitors of human papillomavirus oncoprotein E6

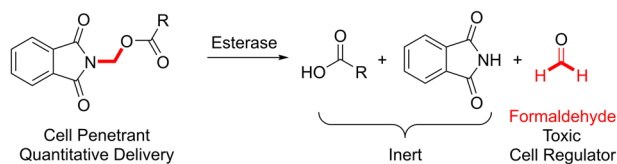
Xiyun Ye, Peiyuan Zhang, Jason Tao, John C. K. Wang, Amirhossein Mafi, Nathalie M. Grob, Anthony J. Quartararo, Hannah T. Baddock, Leanne J. G. Chan, Fiona E. McAllister, Ian Foe, Andrei Loas, Dan L. Eaton, Qi Hao, Aaron H. Nile* and Bradley L. Pentelute*



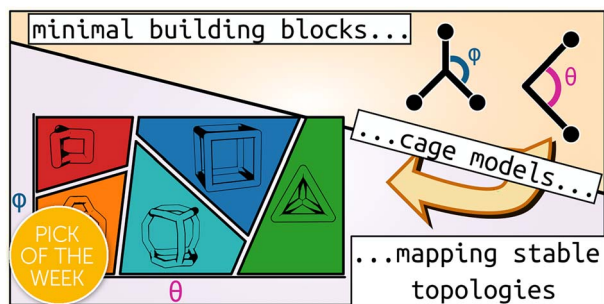
12498

N-Acyloxymethyl-phthalimides deliver genotoxic formaldehyde to human cells

Vicki L. Emms, Liam A. Lewis, Lilla Beja, Natasha F. A. Bulman, Elisabete Pires, Frederick W. Muskett, James S. O. McCullagh, Lonnie. P. Swift,* Peter J. McHugh* and Richard J. Hopkinson*



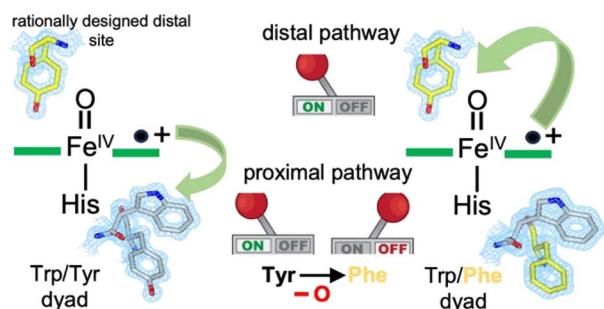
12506



Systematic exploration of accessible topologies of cage molecules *via* minimalistic models

Andrew Tarzia,* Emma H. Wolpert, Kim E. Jelfs and Giovanni M. Pavan*

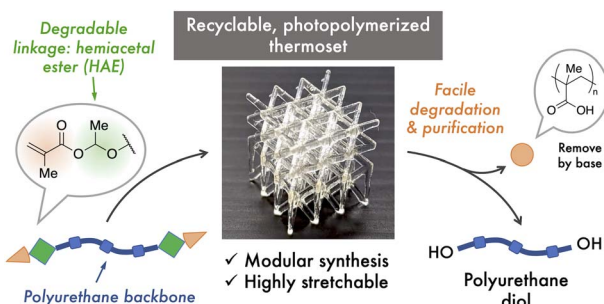
12518



New insights into controlling radical migration pathways in heme enzymes gained from the study of a dye-decolorising peroxidase

Marina Lučić, Michael T. Wilson, Jacob Pullin, Michael A. Hough, Dimitri A. Svistunenko* and Jonathan A. R. Worrall*

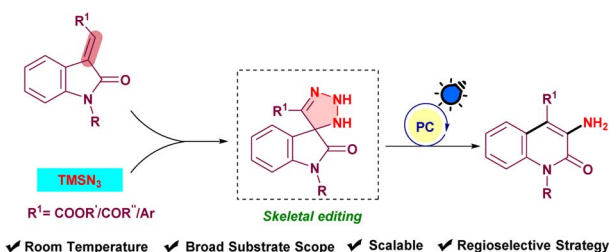
12535



Stretchable, recyclable thermosets *via* photopolymerization and 3D printing of hemiacetal ester-based resins

You-Chi Mason Wu, Gloria Chyr, Hyunchang Park, Anna Makar-Limanov, Yuran Shi, Joseph M. DeSimone and Zhenan Bao*

12541



Skeletal rearrangement through photocatalytic denitrogenation: access to C-3 aminoquinolin-2(1H)-ones

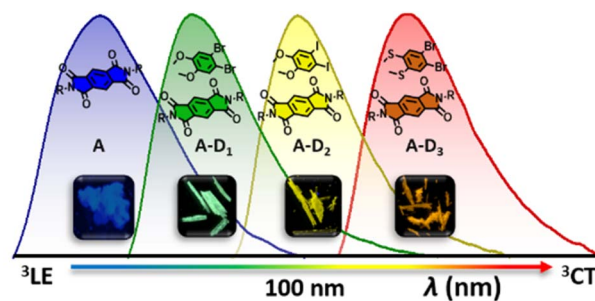
Swati Singh, Gopal Chakraborty and Sudipta Raha Roy*



12548

Revisiting organic charge-transfer cocrystals for wide-range tunable, ambient phosphorescence

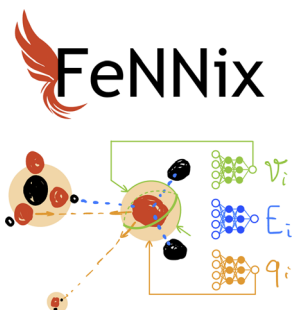
Anju Ajayan Kongasseri, Shagufi Naz Ansari, Swadhin Garain, Sopan M. Wagalgave and Subi J. George*



12554

Force-field-enhanced neural network interactions: from local equivariant embedding to atom-in-molecule properties and long-range effects

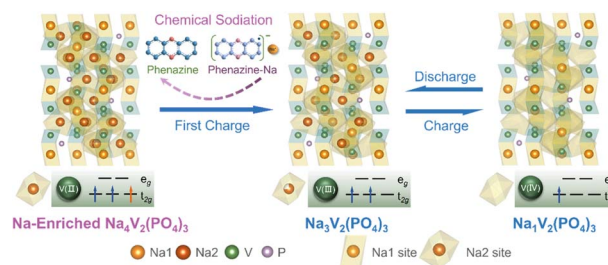
Thomas Plé,* Louis Lagardère* and Jean-Philip Piquemal*



12570

Controllable synthesis of a Na-enriched $\text{Na}_4\text{V}_2(\text{PO}_4)_3$ cathode for high-energy sodium-ion batteries: a redox-potential-matched chemical sodiation approach

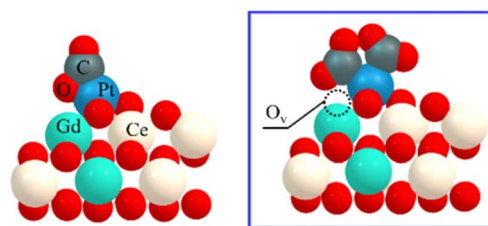
Mingli Xu, Fengxue Zhang, Yanhui Zhang, Chen Wu, Xue Zhou, Xiping Ai and Jiangfeng Qian*



12582

Active sites of atomically dispersed Pt supported on Gd-doped ceria with improved low temperature performance for CO oxidation

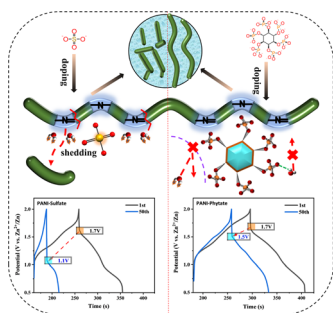
Yuanyuan Li,* Haodong Wang, Haohong Song, Ning Rui, Matthew Kottwitz, Sanjaya D. Senanayake, Ralph G. Nuzzo, Zili Wu, De-en Jiang and Anatoly I. Frenkel*



- Improved CO oxidation
- Different mechanism



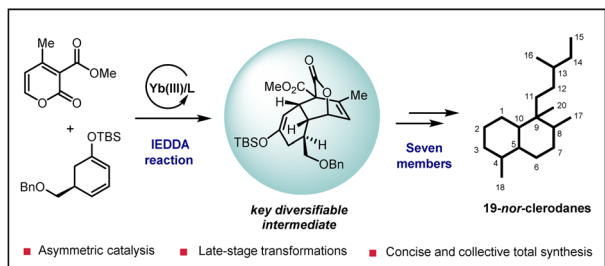
12589



Enhancing organic cathodes of aqueous zinc-ion batteries via utilizing steric hindrance and electron cloud equalization

Guanzhong Ma, Zhengyu Ju, Xin Xu, Yunfei Xu, Yao Sun, Yaqun Wang,* Guoxin Zhang, Mian Cai, Lijia Pan* and Guihua Yu*

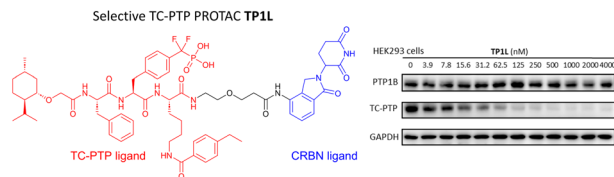
12598



Enantioselective and collective total synthesis of pentacyclic 19-nor-clerodanes

Zhi-Mao Zhang, Junliang Zhang and Quan Cai*

12606

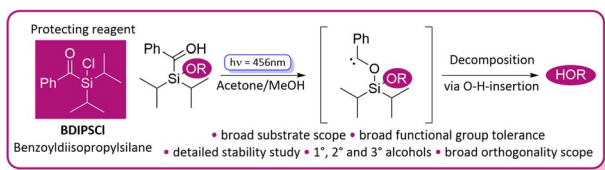


- ✓ $DC_{50} = 35.8$ nM for TC-PTP, > 110-fold selectivity over PTP1B;
- ✓ Elevates pJAK1, pSTAT1, and pLCK levels in cells;
- ✓ Promotes tumor antigen presentation;
- ✓ Enhances T-cell activation and CAR-T cell efficiency.

Discovery of a selective TC-PTP degrader for cancer immunotherapy

Jinmin Miao, Jiajun Dong, Yiming Miao, Yunpeng Bai, Zihan Qu, Brenson A. Jassim, Bo Huang, Quyen Nguyen, Yuan Ma, Allison A. Murray, Jinyue Li, Philip S. Low and Zhong-Yin Zhang*

12615



Benzoyldiisopropylchlorosilane: a visible light photocleavable alcohol protecting group

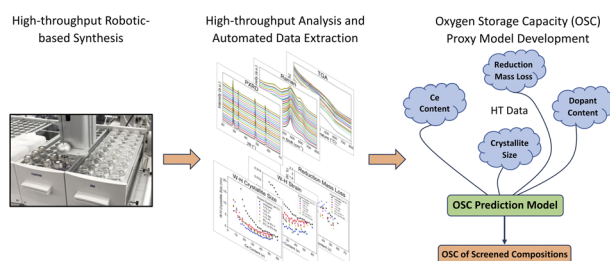
Florian Lind, Kirill Markelov and Armido Studer*



12621

A proxy for oxygen storage capacity from high-throughput screening and automated data analysis

Jack J. Quayle, Alexandros P. Katsoulidis, John B. Claridge, Andrew P. E. York, David Thompsett and Matthew J. Rosseinsky*

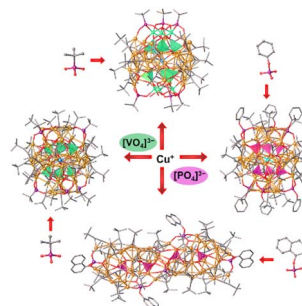


Accelerated discovery of high OSC Materials through high-throughput synthesis, analysis, and proxy models.

12637

Template-assisted synthesis of isomeric copper(i) clusters with tunable structures showing photophysical and electrochemical properties

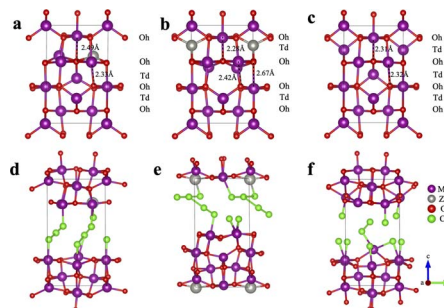
Jun-Jie Fang, Zheng Liu, Yang-Lin Shen, Yun-Peng Xie* and Xing Lu*



12645

Reversible Cl/Cl⁻ redox in a spinel Mn₃O₄ electrode

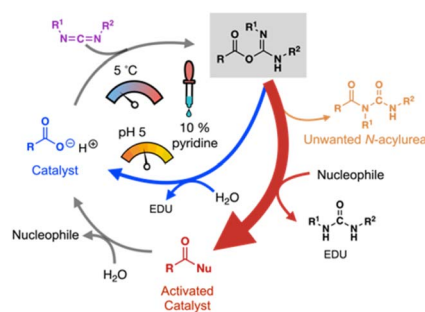
Sean K. Sandstrom, Qiuyao Li, Yiming Sui, Mason Lyons, Chun-Wai Chang, Rui Zhang, Heng Jiang, Mingliang Yu, David Hoang, William F. Stickle, Huolin L. Xin,* Zhenxing Feng,* De-en Jiang* and Xiulei Ji*



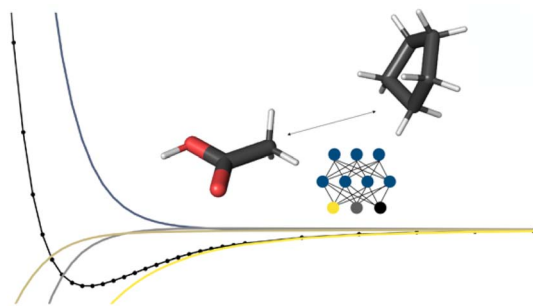
12653

Suppressing catalyst poisoning in the carbodiimide-fueled reaction cycle

Xiaoyao Chen, Héctor Soria-Carrera, Oleksii Zozulia and Job Boekhoven*



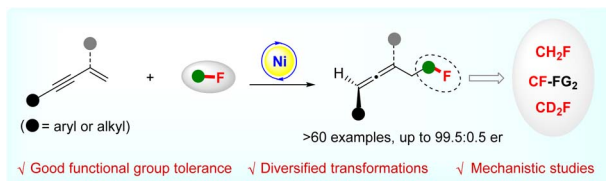
12661



Hybrid classical/machine-learning force fields for the accurate description of molecular condensed-phase systems

Moritz Thürlemann and Sereina Riniker*

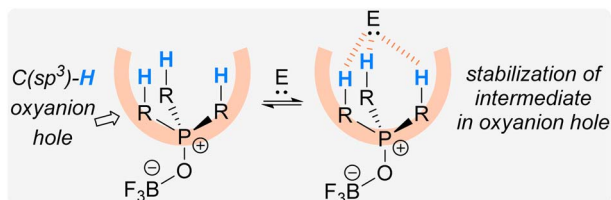
12676



Nickel-catalysed asymmetric hydromonofluoromethylation of 1,3-enynes for enantioselective construction of monofluoromethyl-tethered chiral allenes

Ying Zhang, Jimin Yang, Yu-Long Ruan, Ling Liao, Chuang Ma, Xiao-Song Xue* and Jin-Sheng Yu*

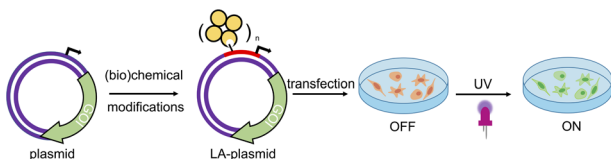
12684



Trialkylphosphonium oxoborates as $C(sp^3)\text{-H}$ oxanion holes and their application in catalytic chemoselective acetalization

Vincent Ming-Yau Leung, Hong-Chai Fabio Wong, Chun-Man Pook, Ying-Lung Steve Tse* and Ying-Yeung Yeung*

12693



Sequence-independent, site-specific incorporation of chemical modifications to generate light-activated plasmids

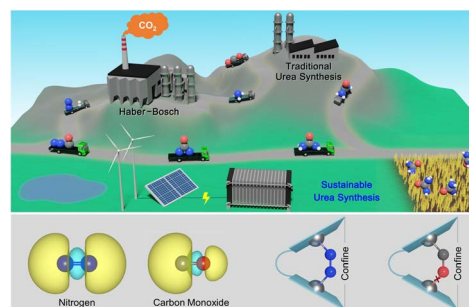
Khoa Chung and Michael J. Booth*



12707

Steering competitive N_2 and CO adsorption toward efficient urea production with a confined dual site

Zhe Chen, Yonghua Liu and Tao Wang*

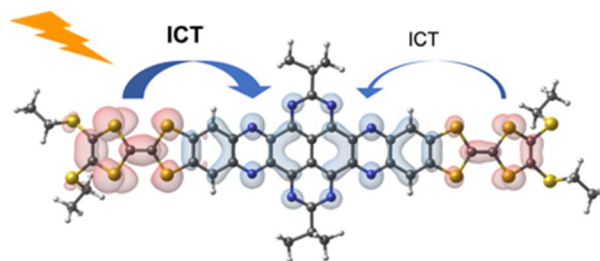


12715

Photoinduced asymmetric charge trapping in a symmetric tetraazapyrene-fused bis(tetrathiafulvalene) conjugate

Ping Zhou, Maryam Nazari Haghighi Pashaki, Hans-Martin Frey, Andreas Hauser, Silvio Decurtins, Andrea Cannizzo,* Thomas Feurer, Robert Häner, Ulrich Aschauer* and Shi-Xia Liu*

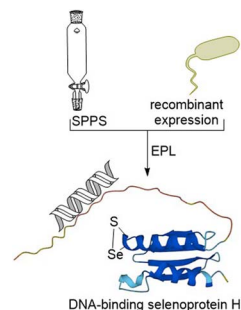
Asymmetric Charge Trapping via Electrostatic Stabilization



12723

The semisynthesis of nucleolar human selenoprotein H

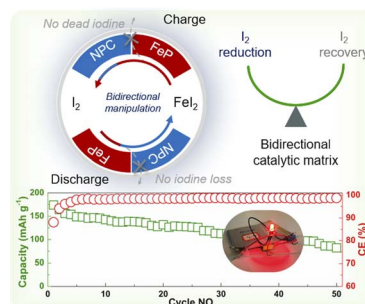
Rebecca Notis Dardashti, Shay Laps, Jacob S. Gichtin and Norman Metanis*



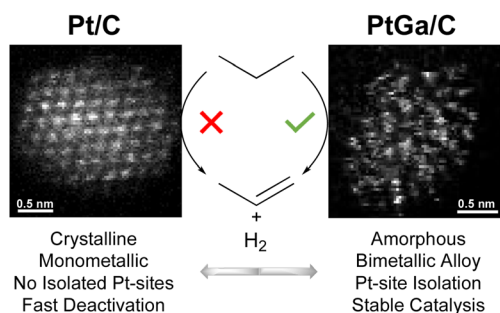
12730

Bidirectional manipulation of iodine redox kinetics in aqueous $Fe-I_2$ electrochemistry

Weiwei Zhang, Mingli Wang, Hong Zhang,* Lin Fu, Wenli Zhang, Yupeng Yuan* and Ke Lu*



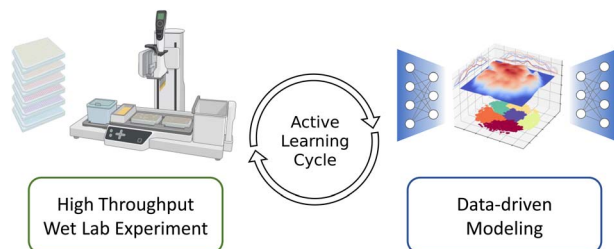
12739



Implications of Ga promotion and metal–oxide interface from tailored PtGa propane dehydrogenation catalysts supported on carbon

Enzo Brack, Milivoj Plodinec, Marc-Georg Willinger and Christophe Copéret*

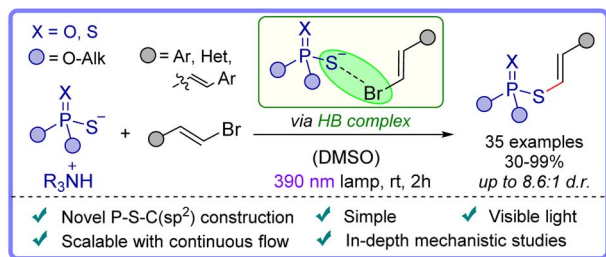
12747



Data-driven discovery of innate immunomodulators via machine learning-guided high throughput screening

Yifeng Tang, Jeremiah Y. Kim, Carman K. M. IP, Azadeh Bahmani, Qing Chen, Matthew G. Rosenberger, Aaron P. Esser-Kahn* and Andrew L. Ferguson*

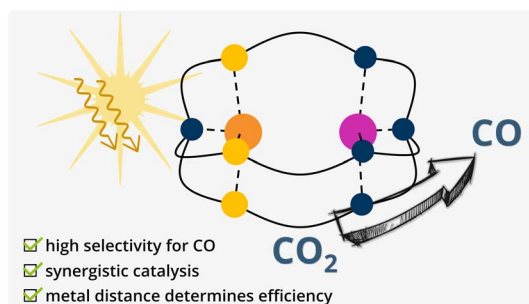
12767



Photochemical halogen-bonding assisted carbothiophosphorylation reactions of alkenyl and 1,3-dienyl bromides

Helena F. Piedra, Victoria Gebler, Carlos Valdés and Manuel Plaza*

12774



A Cu^I/Co^{II} cryptate for the visible light-driven reduction of CO₂

Julia Jökel, Esma Birsan Boydas, Joël Wellauer, Oliver S. Wenger, Marc Robert, Michael Römelts* and Ulf-Peter Apfel*

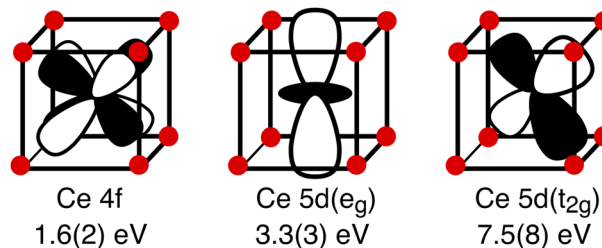


EDGE ARTICLES

12784

Strengths of covalent bonds in LnO₂ determined from O K-edge XANES spectra using a Hubbard model

Wayne W. Lukens, Jr.,* Stefan G. Minasian and Corwin H. Booth



CORRECTION

12796

Correction: Fast and scalable solvent-free access to Lappert's heavier tetrylenes E{N(SiMe₃)₂}₂ (E = Ge, Sn, Pb) and ECl{N(SiMe₃)₂} (E = Ge, Sn)

Javier A. Cabeza, Javier F. Reynes, Felipe García,* Pablo García-Álvarez* and Rubén García-Soriano

