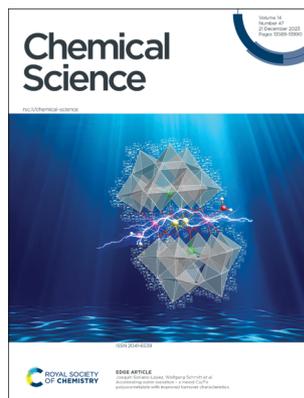


IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(47) 13589–13990 (2023)



Cover
See Iria Bolaño Losada and Petter Persson, pp. 13713–13721. Image reproduced by permission of Iria Bolaño Losada from *Chem. Sci.*, 2023, **14**, 13713. Artwork by Iria Bolaño Losada.



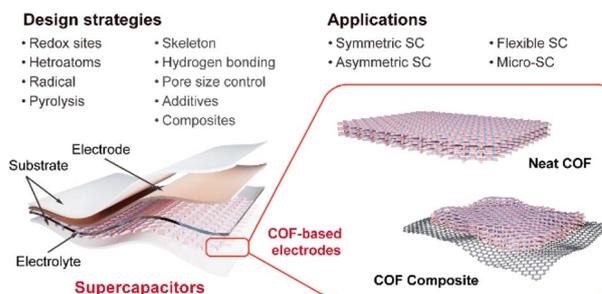
Inside cover
See Joaquín Soriano-López, Wolfgang Schmitt et al., pp. 13722–13733. Image reproduced by permission of Joaquín Soriano-López and Juan José Mufanó from *Chem. Sci.*, 2023, **14**, 13722.

REVIEWS

13601

Recent advances in the utilization of covalent organic frameworks (COFs) as electrode materials for supercapacitors

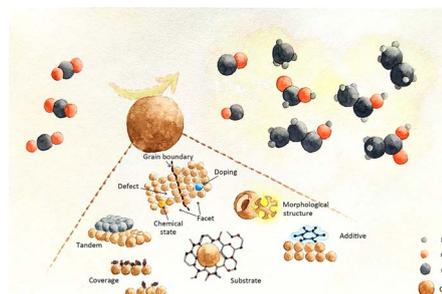
Shen Xu, Jinghang Wu, Xiang Wang and Qichun Zhang*



13629

Cu-based catalyst designs in CO₂ electroreduction: precise modulation of reaction intermediates for high-value chemical generation

Liangyiqun Xie, Yujing Jiang, Wenlei Zhu, Shichao Ding, Yang Zhou* and Jun-Jie Zhu*



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, MPIK
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, 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

Editorial Staff

Executive Editor

May Copsey

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 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

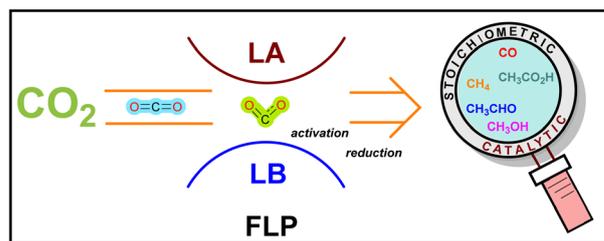


REVIEWS

13661

Advances in CO₂ activation by frustrated Lewis pairs: from stoichiometric to catalytic reactions

Md. Nasim Khan, Yara van Ingen, Tribani Boruah, Adam McLauchlan, Thomas Wirth* and Rebecca L. Melen*

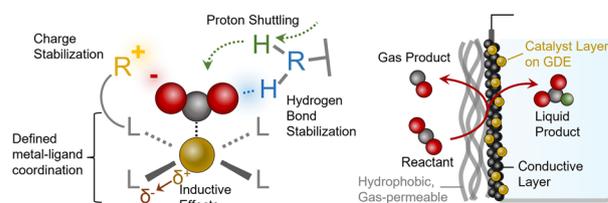


PERSPECTIVE

13696

Electrocatalysis with molecules and molecular assemblies within gas diffusion electrodes

Hossein Bemana, Morgan McKee and Nikolay Kornienko*

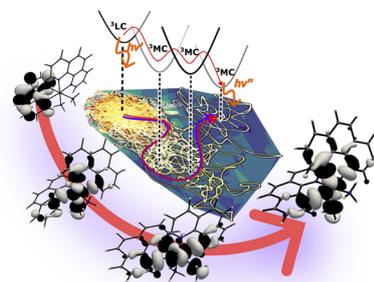


EDGE ARTICLES

13713

Ligand-centered to metal-centered activation of a Rh(III) photosensitizer revealed by *ab initio* molecular dynamics simulations

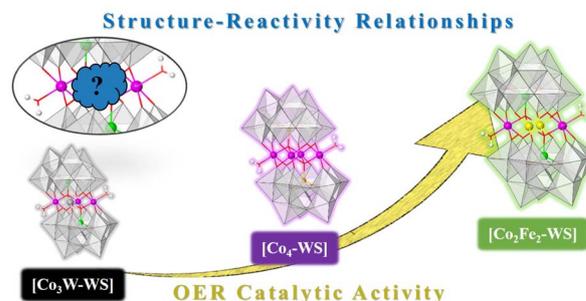
Iria Bolaño Losada and Petter Persson*



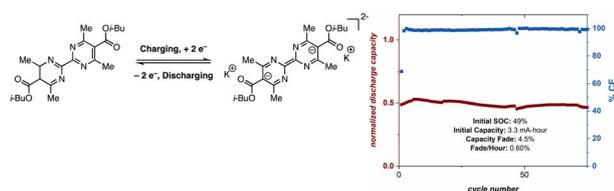
13722

Accelerating water oxidation – a mixed Co/Fe polyoxometalate with improved turnover characteristics

Joaquín Soriano-López,* Friedrich W. Steuber, Muhamed Mulahmetović, Maria Besora, Juan Modesto Clemente-Juan, Mariah O'Doherty, Nian-Yong Zhu, Craig L. Hill, Eugenio Coronado, Josep M. Poble and Wolfgang Schmitt*



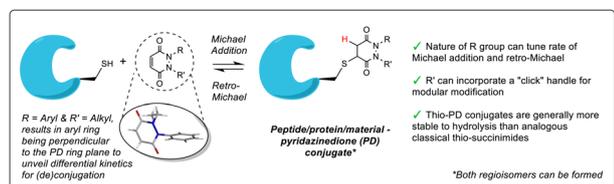
13734



Data science enabled discovery of a highly soluble 2,2'-bipyrimidine anolyte for application in a flow battery

Adam R. Pancoast, Sara L. McCormack, Shelby Galinat, Ryan Walser-Kuntz, Brianna M. Jett, Melanie S. Sanford and Matthew S. Sigman*

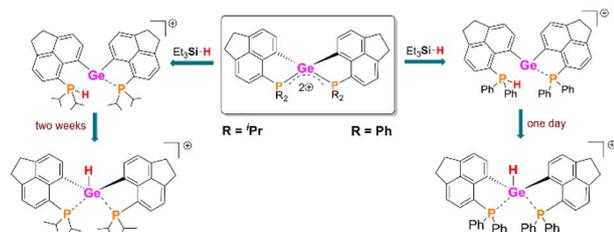
13743



Use of pyridazinediones for tuneable and reversible covalent cysteine modification applied to peptides, proteins and hydrogels

Léa N. C. Rochet, Calise Bahou, Jonathan P. Wojciechowski, Ilias Koutsopeiras, Phyllida Britton, Richard J. Spears, Ioanna A. Thanasi, Baihao Shao, Lisha Zhong, Dejan-Krešimir Bučar, Abil E. Aliev, Michael J. Porter, Molly M. Stevens, James R. Baker* and Vijay Chudasama*

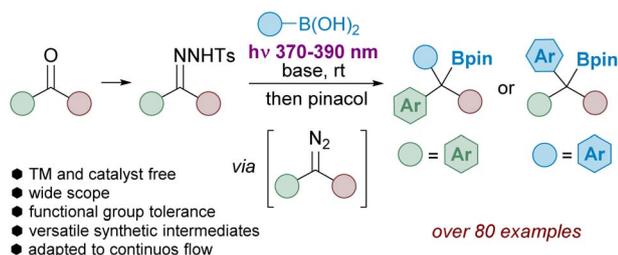
13755



Intramolecular donor-stabilized tetra-coordinated germanium(IV) di-cations and their Lewis acidic properties

Balakrishna Peddi, Souvik Khan, Rajesh G. Gonnade, Cem B. Yildiz* and Moumita Majumdar*

13765



Synthesis of substituted benzylboronates by light promoted homology of boronic acids with N-sulfonylhydrazones

Álvaro Valdés-Maqueda, Lucía López, Manuel Plaza* and Carlos Valdés*

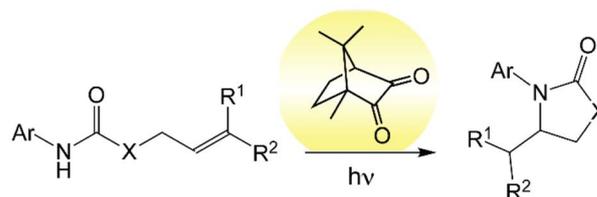


13776

Chemoselective bond activation by unidirectional and asynchronous PCET using ketone photoredox catalysts

Rui Sun, Serge Ruccolo, Daniel L. Nascimento, Yangzhong Qin, Nathaniel Hibbert and Daniel G. Nocera*

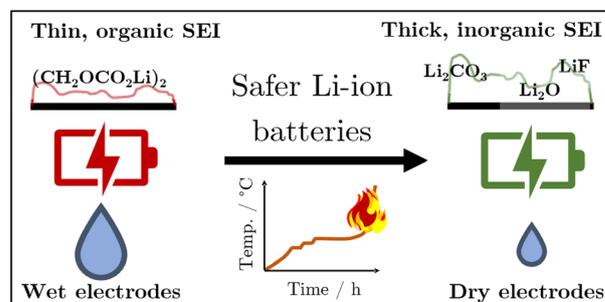
- ✓ Base-free
- ✓ Non-toxic
- ✓ Inexpensive
- ✓ Biocompatible



13783

Impact of electrolyte impurities and SEI composition on battery safety

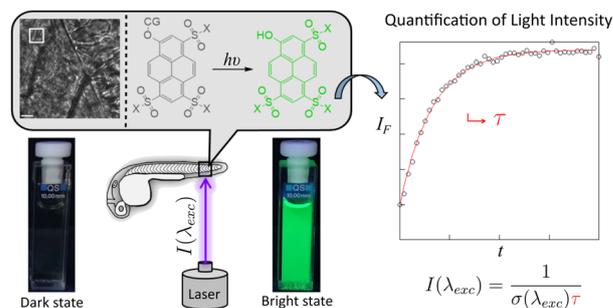
Florian Baakes, Daniel Witt and Ulrike Krewer*



13799

A series of caged fluorophores for calibrating light intensity

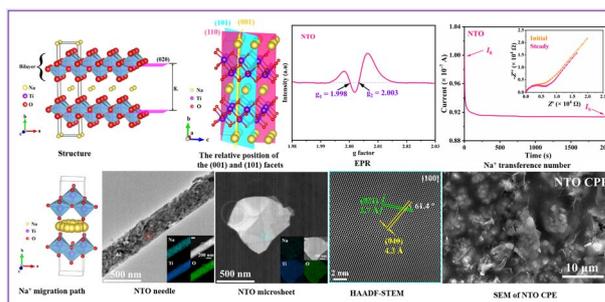
Mrinal Mandal, Hessam Sepasi Tehrani, Qianhua Mai, Emma Simon, Marie-Aude Plamont, Christine Rampon, Sophie Vrız, Isabelle Aujard,* Thomas Le Saux* and Ludovic Jullien*



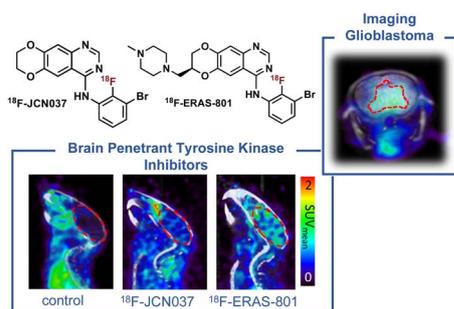
13812

Layered sodium titanate with a matched lattice: a single ion conductor in a solid-state sodium metal battery

Xuanao Ma, Yang Liu, Yunhuai Zhang and Yun Gong*



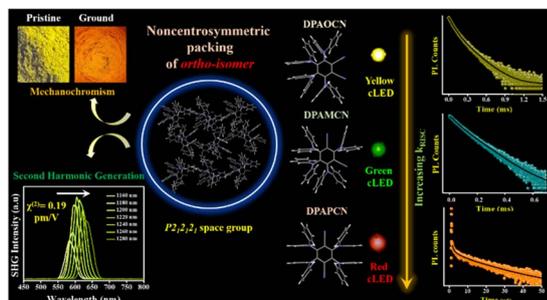
13825



^{18}F -Labeled brain-penetrant EGFR tyrosine kinase inhibitors for PET imaging of glioblastoma

Maruthi Kumar Narayanam, Jonathan E. Tsang, Shili Xu, David A. Nathanson and Jennifer M. Murphy*

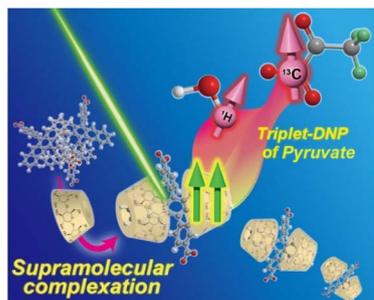
13832



Engineering TADF, mechanochromism, and second harmonic up-conversion properties in regioisomeric substitution space

Abhijit Chatterjee, Joy Chatterjee, Subrahmanyam Sappati, Riteeka Tanwar, Madan D. Ambhore, Habibul Arfin, Rintu M. Umesh, Mayurika Lahiri, Pankaj Mandal and Partha Hazra*

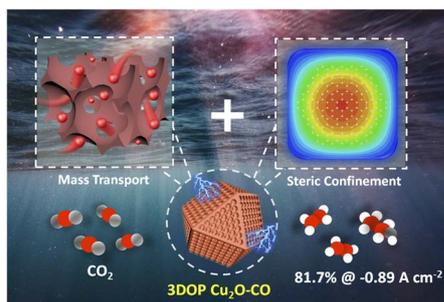
13842



Triplet dynamic nuclear polarization of pyruvate via supramolecular chemistry

Tomoyuki Hamachi, Koki Nishimura, Keita Sakamoto, Yusuke Kawashima, Hironori Kouno, Shunsuke Sato, Go Watanabe, Kenichiro Tateishi, Tomohiro Uesaka and Nobuhiro Yanai*

13851



Evoking C_2^+ production from electrochemical CO_2 reduction by the steric confinement effect of ordered porous Cu_2O

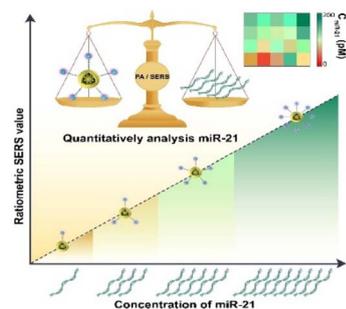
Longlong Fan, Qinghong Geng, Lian Ma, Chengming Wang, Jun-Xuan Li, Wei Zhu, Ruiwen Shao, Wei Li, Xiao Feng, Yusuke Yamauchi, Cuiling Li* and Lei Jiang



13860

Quantitative detection of microRNA-21 *in vivo* using *in situ* assembled photoacoustic and SERS nanoprobe

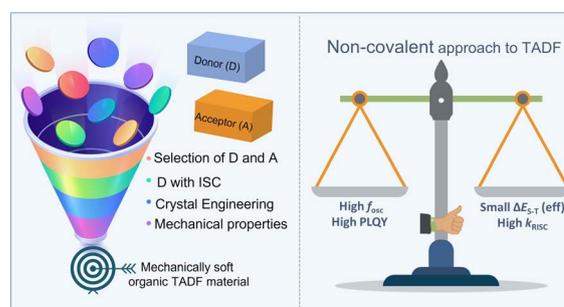
Liting Zheng, Qingqing Li, Ying Wu, Lichao Su, Wei Du, Jibin Song, Lanlan Chen* and Huanghao Yang*



13870

Thermally activated delayed fluorescence in a mechanically soft charge-transfer complex: role of the locally excited state

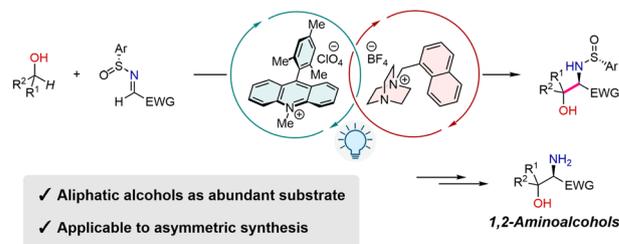
Kalyan Jyoti Kalita, Saikat Mondal, C. Malla Reddy* and Ratheesh K. Vijayaraghavan*



13879

Facile synthesis of 1,2-aminoalcohols via α -C-H aminoalkylation of alcohols by photoinduced hydrogen-atom transfer catalysis

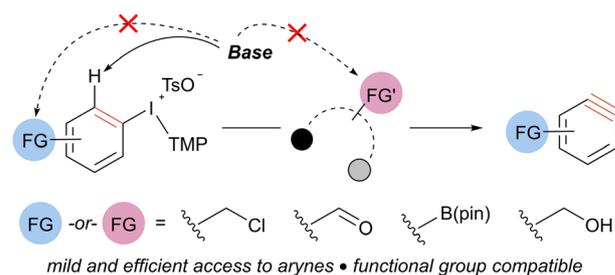
Joaquim Caner, Akira Matsumoto* and Keiji Maruoka*



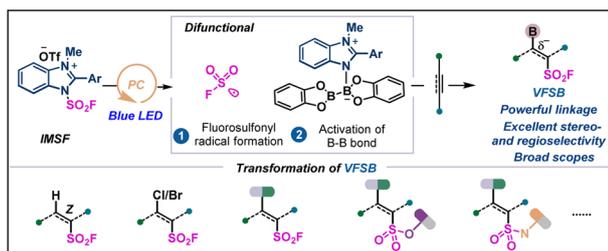
13885

An efficient and chemoselective method to generate arynes

Bryan E. Metzger, Riley A. Roberts, Aleksandra Nilova and David R. Stuart*



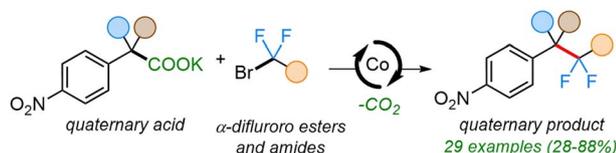
13893



Photoredox-catalyzed stereo- and regioselective vicinal fluorosulfonyl-borylation of unsaturated hydrocarbons

Heyin Li, Mengjun Huang, Zhenlei Zou, Zhen Wang, Yifan Li, Chao Sun, Wangzhe Chen, Yi Pan, Weigang Zhang* and Yi Wang*

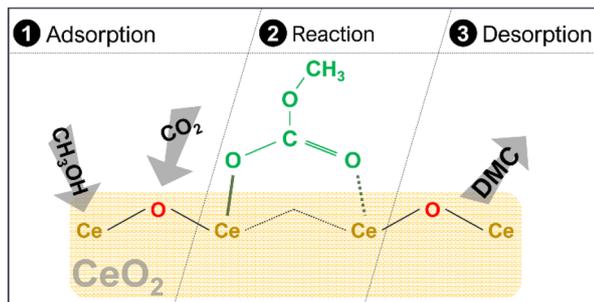
13902



Cobalt-catalyzed decarboxylative difluoroalkylation of nitrophenylacetic acid salts

Ebbin Joseph, Ian Smith and Jon A. Tunge*

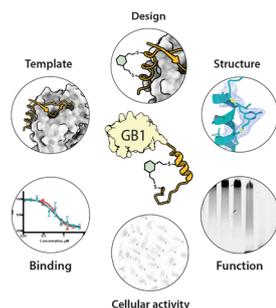
13908



Dimethyl carbonate synthesis from CO₂ and methanol over CeO₂: elucidating the surface intermediates and oxygen vacancy-assisted reaction mechanism

Dragos Stoian, Toshiyuki Sugiyama, Atul Bansode, Francisco Medina, Wouter van Beek, Jun-ya Hasegawa, Akira Nakayama* and Atsushi Urakawa*

13915



A recombinant approach for stapled peptide discovery yields inhibitors of the RAD51 recombinase

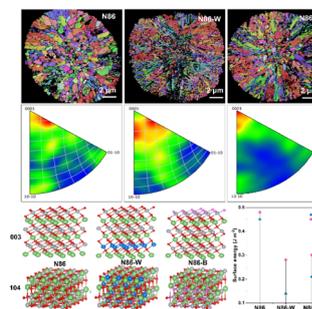
Teodors Pantelejevs,* Pedro Zuazua-Villar, Oliwia Koczy, Andrew J. Counsell, Stephen J. Walsh, Naomi S. Robertson, David R. Spring, Jessica A. Downs and Marko Hyvönen*



13924

Manipulating the crystal plane angle within the primary particle arrangement for the radial ordered structure in a Ni-rich cathode

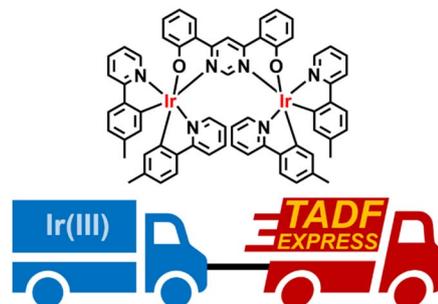
Ting Chen, Chuyao Wen, Chen Wu, Lang Qiu, Zhenguo Wu,* Jiayang Li, Yanfang Zhu, Haoyu Li, Qingquan Kong, Yang Song, Fang Wan, Mingzhe Chen, Ismael Saadoun, Benhe Zhong, Shixue Dou, Yao Xiao* and Xiaodong Guo*



13934

Thermally activated delayed fluorescence in a deep red dinuclear iridium(III) complex: a hidden mechanism for short luminescence lifetimes

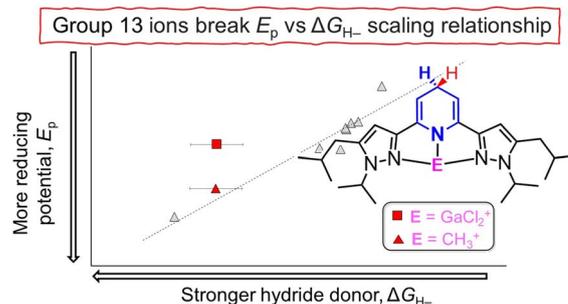
Piotr Pander,* Andrey V. Zaytsev, Amit Sil, Glib V. Baryshnikov, Farhan Siddique, J. A. Gareth Williams,* Fernando B. Dias* and Valery N. Kozhevnikov*



13944

Group 13 ion coordination to pyridyl breaks the reduction potential vs. hydricity scaling relationship for dihydropyridinates

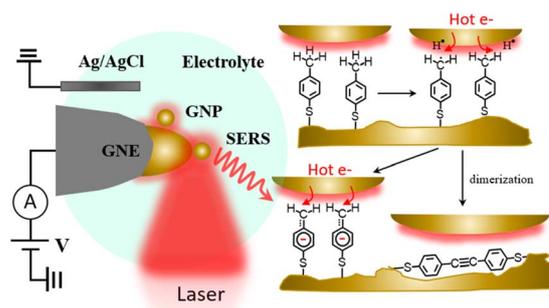
Leo W. T. Parsons, James C. Fettinger and Louise A. Berben*



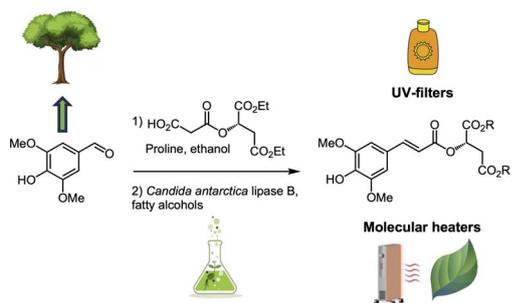
13951

Plasmon-mediated dehydrogenation of the aromatic methyl group and benzyl radical formation

Jianghao Zhou, Jing Guo, Govinda Ghimire, Alexander M. Mebel, Shuai Chang* and Jin He*



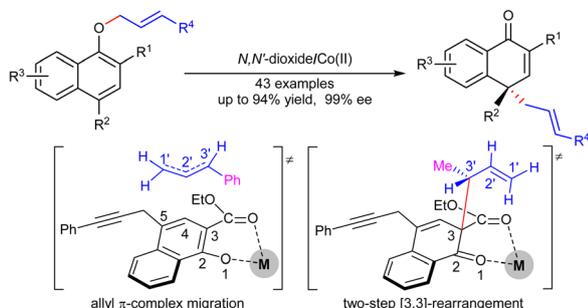
13962



An expeditive and green chemo-enzymatic route to diester sinapoyl-L-malate analogues: sustainable bioinspired and biosourced UV filters and molecular heaters

Benjamin Rioux, Louis M. M. Mouterde, Jimmy Alarcán, Temitope T. Abiola, Matthias J. A. Vink, Jack M. Woolley, Aurélien A. M. Peru, Matthieu M. Mention, Fanny Brunissen, Giel Berden, Jos Oomens,* Albert Braeuning,* Vasilios G. Stavros* and Florent Allais*

13979



Chiral cobalt(II) complex-promoted asymmetric *para*-Claisen rearrangement of allyl α -naphthol ethers

Hongkun Zeng, Lifeng Wang, Zhishan Su, Meijia Ying, Lili Lin* and Xiaoming Feng*

CORRECTIONS

13986

Correction: A non-sacrificial method for the quantification of poly(ethylene glycol) grafting density on gold nanoparticles for applications in nanomedicine

Jun Lu, Yao Xue, Rui Shi, Jing Kang, Chao-Yang Zhao, Ning-Ning Zhang, Chun-Yu Wang, Zhong-Yuan Lu* and Kun Liu*

13987

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

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

