

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(39) 10615–10982 (2023)



**Cover**  
See Alexander Kuhn, Neso Sojic *et al.*, pp. 10664–10670. Image reproduced by permission of Xiaoqing Yang from *Chem. Sci.*, 2023, 14, 10664.



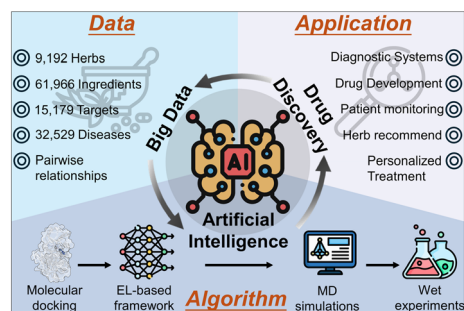
**Inside cover**  
See Jana Selent, Mette Marie Rosenkilde *et al.*, pp. 10671–10683. Image reproduced by permission of Viktoria Madeline Skovgaard Kjær, Tomasz Stepniewski, Mette Rosenkilde and Jana Selent from *Chem. Sci.*, 2023, 14, 10671.

## COMMENTARY

10628

### A focus on harnessing big data and artificial intelligence: revolutionizing drug discovery from traditional Chinese medicine sources

Mingyu Li and Jian Zhang\*

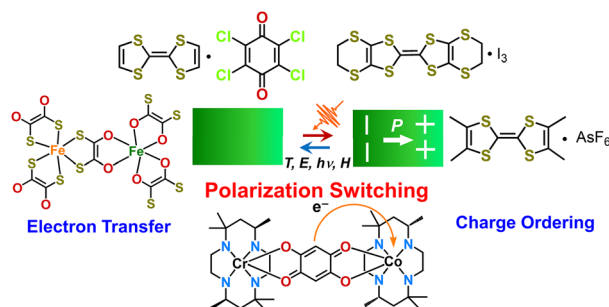


## PERSPECTIVES

10631

### Control of electronic polarization *via* charge ordering and electron transfer: electronic ferroelectrics and electronic pyroelectrics

Sheng-Qun Su, Shu-Qi Wu, Shinji Kanegawa, Kaoru Yamamoto and Osamu Sato\*



# 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  
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  
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, KAIST  
S. Kath-Schorr, University of Cologne  
T. Kato, University of Tokyo  
C. Kelly, Janssen 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. Patel, 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. Reischer, University of Cambridge  
A. Rentmeister, WWU Munster  
J. Rinehart, UC San Diego  
A. Roitberg, University of Florida  
H. Sardon, UPV-EHU  
R. Sarpong, UC Berkeley  
G. Schatz, Northwestern University  
D. Schultz, Merck  
D. Seferos, University of Toronto  
R. Sessoli, University of Florence  
B. 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, NCSST  
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](http://rsc.li/chemical-science)

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

## 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](mailto:chemicalscience@rsc.org)

For pre-submission queries please contact May Copsey, 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)

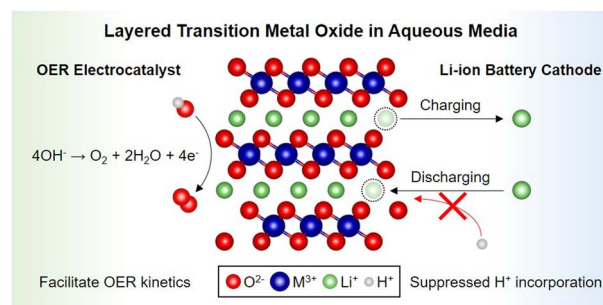


## PERSPECTIVES

10644

## Layered transition metal oxides (LTMO) for oxygen evolution reactions and aqueous Li-ion batteries

Yohan Kim, Eunjin Choi, Seunggu Kim and Hye Ryung Byon\*

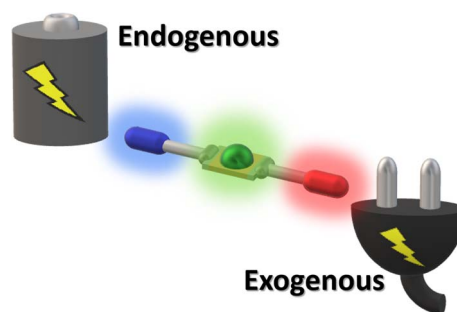


## EDGE ARTICLES

10664

## Endogenous and exogenous wireless multimodal light-emitting chemical devices

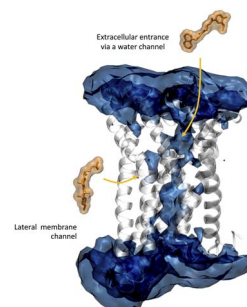
Miaoxia Liu, Gerardo Salinas, Jing Yu, Antoine Cornet, Haidong Li, Alexander Kuhn\* and Neso Sojic\*



10671

## Ligand entry pathways control the chemical space recognized by GPR183

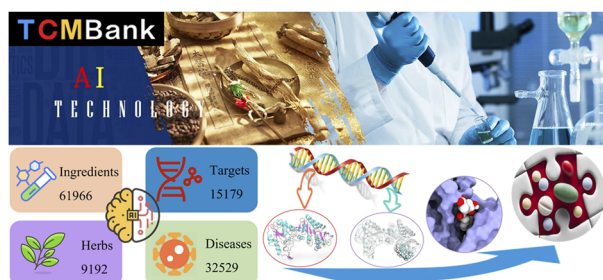
Viktoria Madeline Skovgaard Kjær, Tomasz Maciej Stępniewski, Brian Medel-Lacruz, Lisa Reinmuth, Marija Ciba, Elisabeth Rexen Ulven, Massimiliano Bonomi, Jana Selent\* and Mette Marie Rosenkilde\*



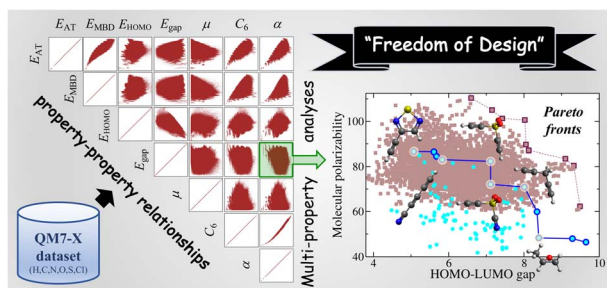
10684

## TCMBank: bridges between the largest herbal medicines, chemical ingredients, target proteins, and associated diseases with intelligence text mining

Qiujie Lv, Guanxing Chen, Haohuai He, Ziduo Yang, Lu Zhao, Hsin-Yi Chen and Calvin Yu-Chian Chen\*



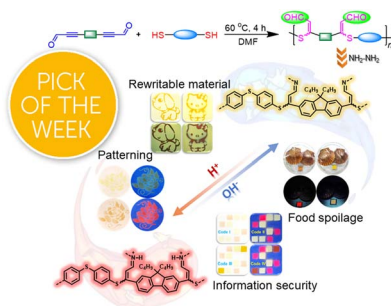
10702



### "Freedom of design" in chemical compound space: towards rational *in silico* design of molecules with targeted quantum-mechanical properties

Leonardo Medrano Sandonas,<sup>\*</sup> Johannes Hoja, Brian G. Ernst, Álvaro Vázquez-Mayagoitia, Robert A. DiStasio, Jr.<sup>\*</sup> and Alexandre Tkatchenko<sup>\*</sup>

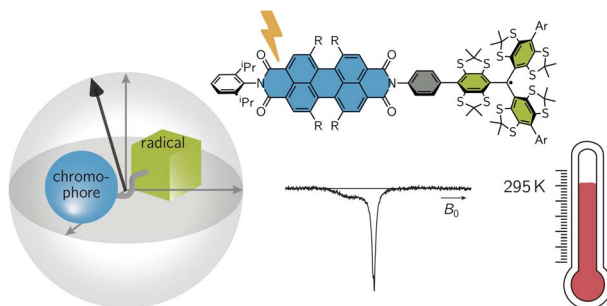
10718



### Acid–base responsive multifunctional poly(formyl sulfide)s through a facile catalyst-free click polymerization of aldehyde-activated internal diynes and dithiols

Baixue Li, Xue Wang, Die Huang, Mingzhao Li, Anjun Qin,<sup>\*</sup> Yusheng Qin<sup>\*</sup> and Ben Zhong Tang

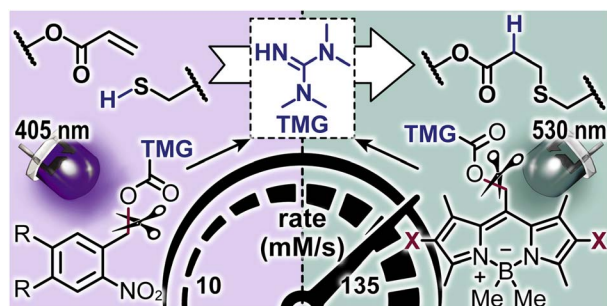
10727



### PDI–trityl dyads as photogenerated molecular spin qubit candidates

Maximilian Mayländer, Kevin Kopp, Oliver Nolden, Michael Franz, Philipp Thielert, Andreas Vargas Jentzsch, Peter Gilch, Olav Schiemann and Sabine Richert<sup>\*</sup>

10736



### Record release of tetramethylguanidine using a green light activated photocage for rapid synthesis of soft materials

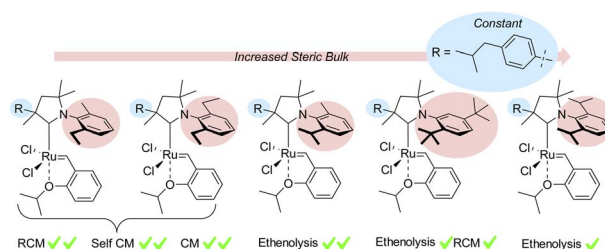
Kun-You Chung, Ain Uddin and Zachariah A. Page<sup>\*</sup>



10744

## A tunable family of CAAC-ruthenium olefin metathesis catalysts modularly derived from a large-scale produced ibuprofen intermediate

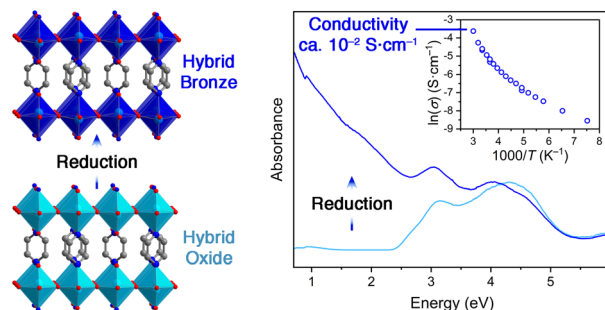
Adrian Sytniczuk, Filip Struzik, Karol Grela and Anna Kajetanowicz\*



10756

## Hybrid bronzes: mixed-valence organic–inorganic metal oxides as a tunable material platform

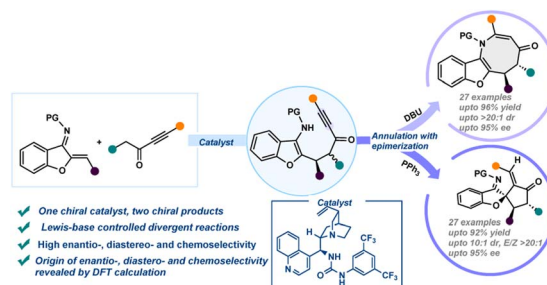
W. Lakna N. Dayaratne, Raúl Torres-Cadena, Bennett P. Schmitt, Emma M. Westrick and Adam Jaffe\*



10768

## Structurally divergent enantioselective synthesis of benzofuran fused azocine derivatives and spirocyclopentanone benzofurans enabled by sequential catalysis

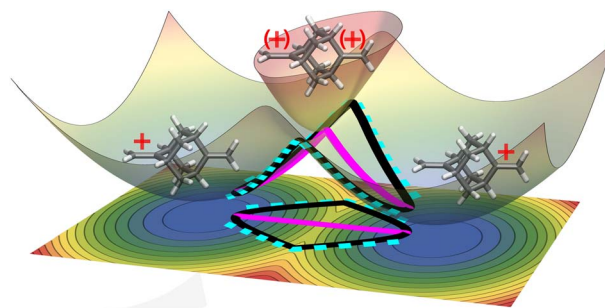
Rupkumar Khuntia, Sanat Kumar Mahapatra, Lisa Roy and Subhas Chandra Pan\*



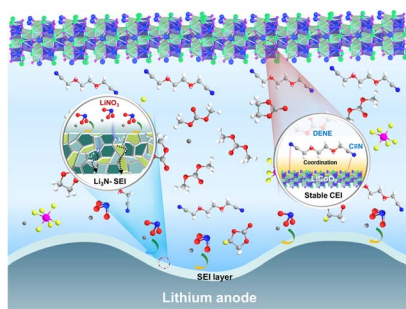
10777

## Competing quantum effects in heavy-atom tunnelling through conical intersections

Wei Fang, Eric R. Heller and Jeremy O. Richardson\*



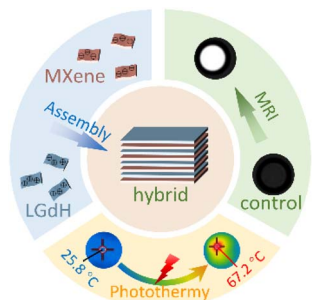
10786



### High-voltage lithium-metal batteries enabled by ethylene glycol bis(propionitrile) ether-LiNO<sub>3</sub> synergistic additives

Shaopeng Li, Kangsheng Huang, Langyuan Wu, Dewei Xiao, Jiang Long, Chenhui Wang, Hui Dou, Pu Chen\* and Xiaogang Zhang\*

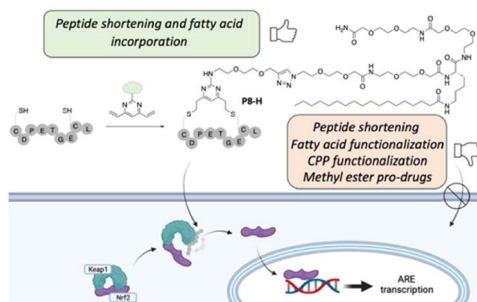
10795



### Rare-earth hydroxide/MXene hybrid: a promising agent for near-infrared phototherapy and magnetic resonance imaging

Mingjun Bai, Linawati Sutrisno, Junhong Duan, Hao Wan,\* Gen Chen, Xiaohe Liu\* and Renzhi Ma\*

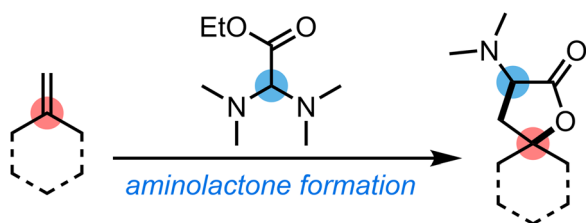
10800



### A cell-active cyclic peptide targeting the Nrf2/Keap1 protein-protein interaction

Jessica Iegre, Sona Krajcovicova, Anders Gunnarsson, Lisa Wissler, Helena Käck, Anna Luchniak, Stefan Tångebjerg, Frank Narjes\* and David R. Spring\*

10806



- aryl-, alkyl-, trisubstituted alkenes
- formation of spirocyclic lactones
- aminogroup can be used for rearrangements

### General acid-mediated aminolactone formation using unactivated alkenes

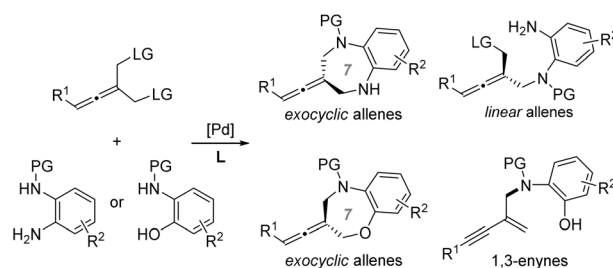
David Just, Carlos R. Gonçalves, Uroš Vezonik, Daniel Kaiser and Nuno Maulide\*



10812

### Chemodivergence in Pd-catalyzed desymmetrization of allenes: enantioselective [4+3] cycloaddition, desymmetric allenylic substitution and enynylation

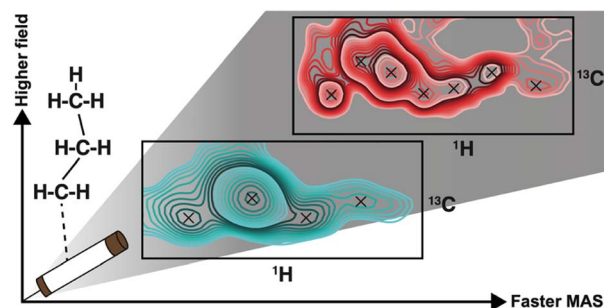
Pengfei Luo, Long Li, Xinfang Mao, Zheng Sun, Yingcheng Wang, Fangzhi Peng and Zhihui Shao\*



10824

### High and fast: NMR protein–proton side-chain assignments at 160 kHz and 1.2 GHz

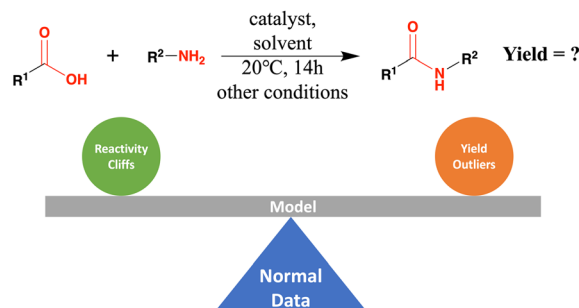
Morgane Callon,\* Dominique Luder, Alexander A. Malär, Thomas Wiegand, Václav Římal, Lauriane Lecoq, Anja Böckmann, Ago Samoson and Beat H. Meier\*



10835

### The challenge of balancing model sensitivity and robustness in predicting yields: a benchmarking study of amide coupling reactions

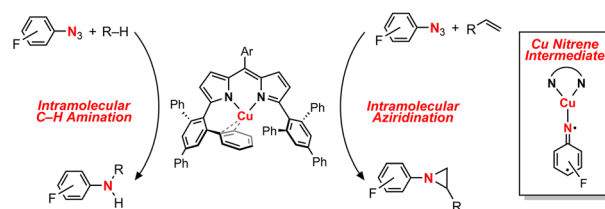
Zhen Liu, Yurii S. Moroz and Olexandr Isayev\*



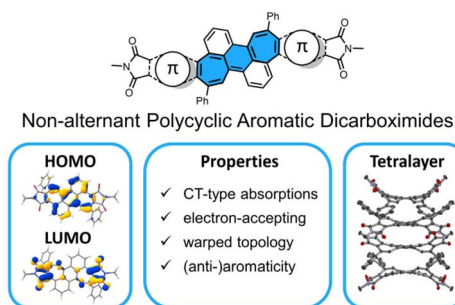
10847

### Nitrene transfer from a sterically confined copper nitrenoid dipyrin complex

Kurtis M. Carsch, Sasha C. North, Ida M. DiMucci, Andrei Iliescu, Petra Vojáčková, Thomas Khazanov, Shao-Liang Zheng, Thomas R. Cundari, Kyle M. Lancaster and Theodore A. Betley\*



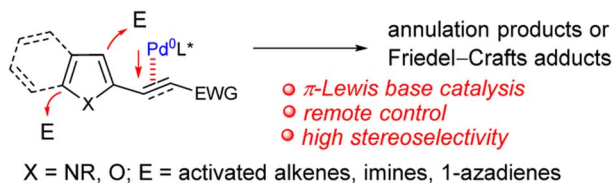
10861



### $\pi$ -Extended benzo[1,2:4,5]di[7]annulene bis(dicarboximide)s – a new class of non-alternant polycyclic aromatic dicarboximides

Jonas Spengler, Chongwei Zhu, Kazutaka Shoyama and Frank Würthner\*

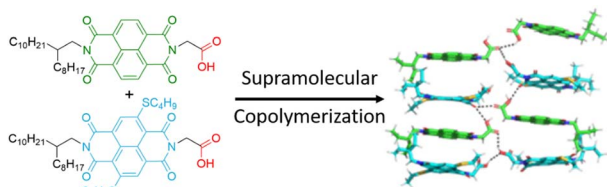
10867



### Asymmetric Friedel–Crafts reaction of unsaturated carbonyl-tethered heteroarenes via vinylogous activation of Pd<sup>0</sup>- $\pi$ -Lewis base catalysis

Bo Jiang, Wu-Tao Gui, Hao-Tian Wang, Ke Xie, Zhi-Chao Chen, Lei Zhu, Qin Ouyang,\* Wei Du\* and Ying-Chun Chen\*

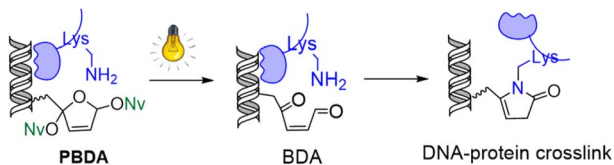
10875



### Supramolecular alternating copolymers with highly efficient fluorescence resonance energy transfer

Anwasha Chakraborty, Pradipta Kumar Das, Biman Jana\* and Suhrit Ghosh\*

10884



### Photo-caged 2-butene-1,4-dial as an efficient, target-specific photo-crosslinker for covalent trapping of DNA-binding proteins

Jiahui Li, Zenghui Cui, Chaochao Fan, Yifei Zhou, Mengtian Ren and Chuangzheng Zhou\*

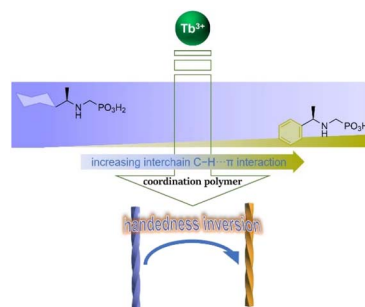
- High specificity for DNA-binding proteins (Lys-rich)
- High photo-crosslinking yields (70%) in minutes



10892

### Macroscopic handedness inversion of terbium coordination polymers achieved by doping homochiral ligand analogues

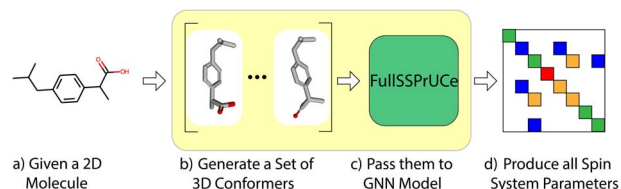
Chang-Yu Wang, Jia-Ge Jia, Guo-Guo Weng, Ming-Feng Qin, Kui Xu and Li-Min Zheng\*



10902

### Rapid prediction of full spin systems using uncertainty-aware machine learning

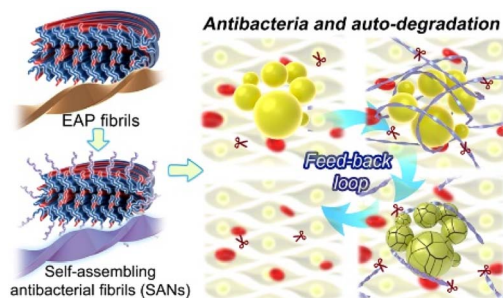
Jake Williams\* and Eric Jonas



10914

### Engineering of antimicrobial peptide fibrils with feedback degradation of bacterial-secreted enzymes

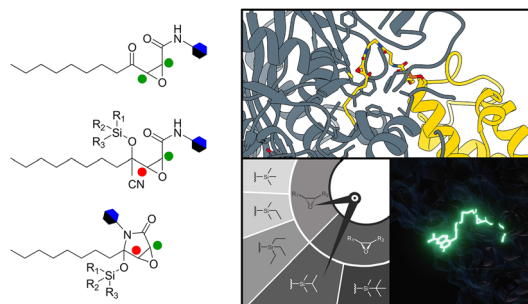
Fenghua Wang, Wencheng Xia, Mingming Zhang, Rongrong Wu, Xiaolu Song, Yun Hao, Yonghai Feng, Liwei Zhang, Dan Li, Wenyan Kang, Cong Liu\* and Lei Liu\*



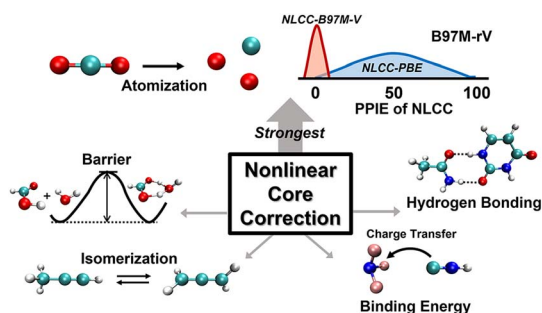
10925

### Masked cerulenin enables a dual-site selective protein crosslink

Ziran Jiang, Aochiu Chen, Jeffrey Chen, Arman Sekhon, Gordon V. Louie, Joseph P. Noel, James J. La Clair and Michael D. Burkart\*



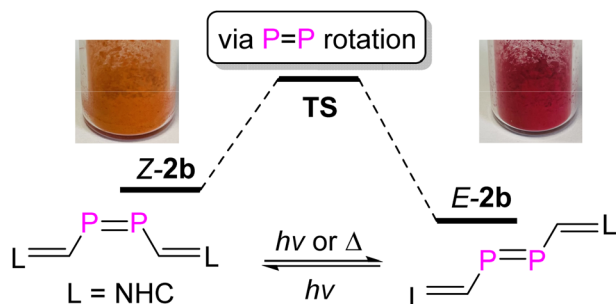
10934



### Greater transferability and accuracy of norm-conserving pseudopotentials using nonlinear core corrections

Wan-Lu Li, Kaixuan Chen, Elliot Rossomme, Martin Head-Gordon and Teresa Head-Gordon\*

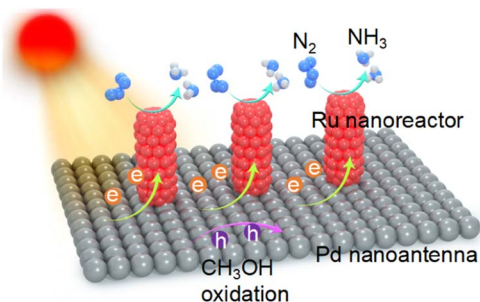
10944



### Room temperature stable *E,Z*-diphosphenes: their isomerization, coordination, and cycloaddition chemistry

Jieli Lin, Shihua Liu, Jie Zhang, Hansjörg Grützmacher, Cheng-Yong Su and Zhongshu Li\*

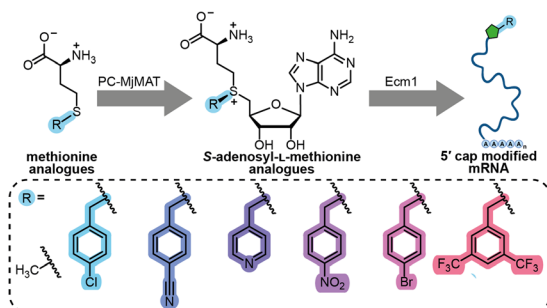
10953



### A Pd-based plasmonic photocatalyst for nitrogen fixation through an antenna–reactor mechanism

Yuanyuan Yang, Henglei Jia,\* Sihua Su, Yidi Zhang, Mengxuan Zhao, Jingzhao Li, Qifeng Ruan\* and Chun-yang Zhang\*

10962



### Post-synthetic benzylation of the mRNA 5' cap via enzymatic cascade reactions

N. V. Cornelissen, R. Mineikaitė, M. Erguven, N. Muthmann, A. Peters, A. Bartels and A. Rentmeister\*

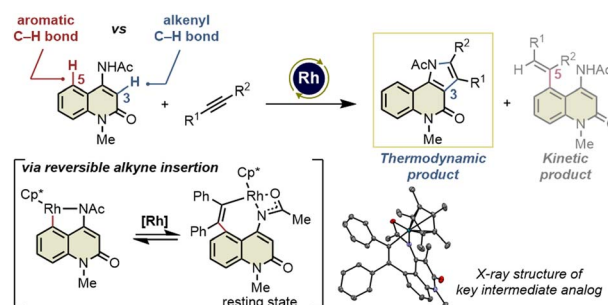


## EDGE ARTICLES

10971

### Rh(III)-catalyzed highly site- and regio-selective alkenyl C–H activation/annulation of 4-amino-2-quinolones with alkynes *via* reversible alkyne insertion

Naohiro Hirako, Takeshi Yasui\* and Yoshihiko Yamamoto\*



## CORRECTION

10979

### Correction: Improving time-resolution and sensitivity of *in situ* X-ray photoelectron spectroscopy of a powder catalyst by modulated excitation

M. Roger, L. Artiglia,\* A. Boucly, F. Buttignol, M. Agote-Arán, J. A. van Bokhoven, O. Kröcher and D. Ferri\*

