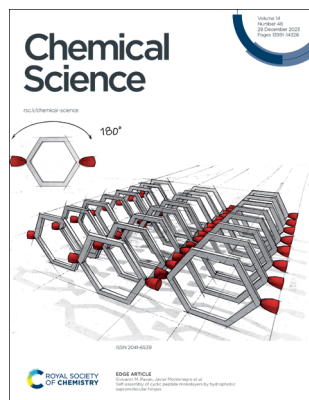


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(48) 13991–14328 (2023)



**Cover**  
See Giovanni M. Pavan, Javier Montenegro *et al.*, pp. 14074–14081. Image reproduced by permission of Beatriz Perez and Javier Montenegro from *Chem. Sci.*, 2023, 14, 14074.



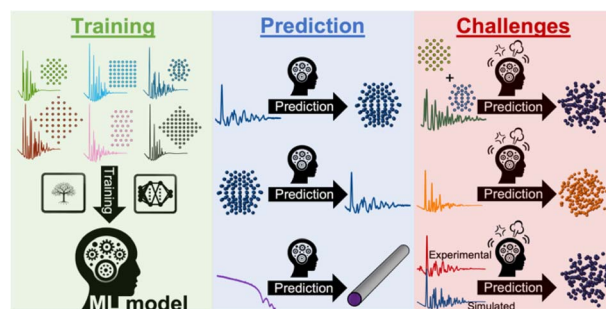
**Inside cover**  
See Andrew Kellett, José Martínez-Costas, Miguel Vázquez López *et al.*, pp. 14082–14091. Image reproduced by permission of M. Eugenio Vázquez from *Chem. Sci.*, 2023, 14, 14082.

## PERSPECTIVES

14003

### Machine learning for analysis of experimental scattering and spectroscopy data in materials chemistry

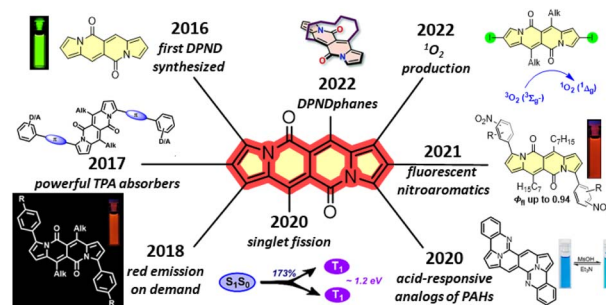
Andy S. Anker, Keith T. Butler, Raghavendra Selvan and Kirsten M. Ø. Jensen\*



14020

### Dipyrrolonaphthyridinedione – (still) a mysterious cross-conjugated chromophore

Bartłomiej Sadowski\* and Daniel T. Gryko\*



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

## Editorial Staff

### Executive Editor

May Copsy

### Deputy Editor

Samantha Apps

### Senior Editor

James Moore

### Scientific Editors

Ellis Crawford, Esther Johnston, Sophie Orchard, Richard Thompson and Amy Welch

### Editorial Assistant

Karina Webster

### Publishing Assistant

David Bishop

For queries about submitted articles please contact James Moore, Senior Editor, in the first instance. E-mail [chemicalscience@rsc.org](mailto:chemicalscience@rsc.org)

For pre-submission queries please contact May Copsy, Executive Editor. E-mail [chemicalscience-rsc@rsc.org](mailto:chemicalscience-rsc@rsc.org)

Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read.

Please email [orders@rsc.org](mailto:orders@rsc.org) to register your interest or contact Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail [orders@rsc.org](mailto:orders@rsc.org)

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

### Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail [advertising@rsc.org](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

## Information for Authors

Full details on how to submit material for publication in Chemical Science are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: [rsc.li/chemical-science](http://rsc.li/chemical-science)

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

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

Registered charity number: 207890

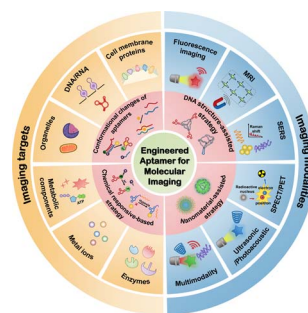


## REVIEWS

14039

**Engineered aptamers for molecular imaging**

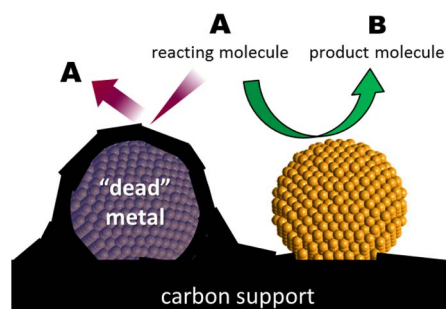
Bingqian Lin,\* Feng Xiao, Jinting Jiang, Zhengjia Zhao and Xiang Zhou



14062

**The phenomenon of “dead” metal in heterogeneous catalysis: opportunities for increasing the efficiency of carbon-supported metal catalysts**

Roman M. Mironenko, Dmitry B. Eremin and Valentine P. Ananikov\*

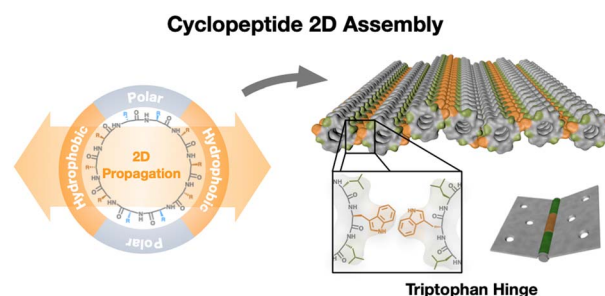


## EDGE ARTICLES

14074

**Self-assembly of cyclic peptide monolayers by hydrophobic supramolecular hinges**

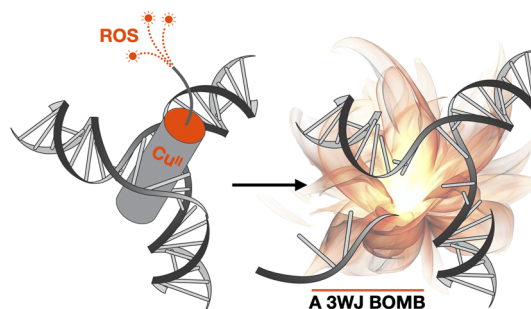
Ignacio Insua, Annalisa Cardellini, Sandra Díaz, Julian Bergueiro, Riccardo Capelli, Giovanni M. Pavan\* and Javier Montenegro\*



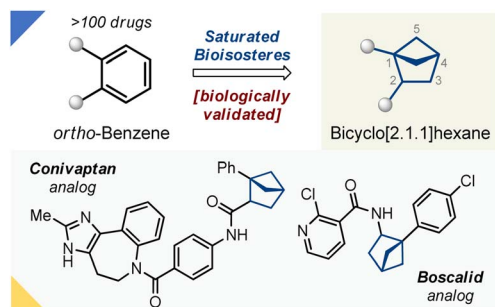
14082

**A copper(II) peptide helicate selectively cleaves DNA replication foci in mammalian cells**

Ana Alcalde-Ordóñez, Natalia Barreiro-Piñeiro, Brionna McGormann, Jacobo Gómez-González, David Bouzada, Francisco Rivadulla, M. Eugenio Vázquez, Andrew Kellett,\* José Martínez-Costas\* and Miguel Vázquez López\*



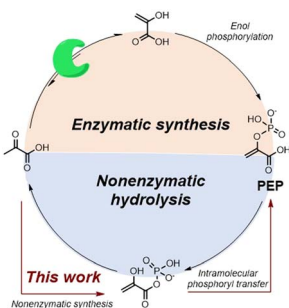
14092



### 1,2-Disubstituted bicyclo[2.1.1]hexanes as saturated bioisosteres of *ortho*-substituted benzene

Aleksandr Denisenko, Pavel Garbuz, Yelyzaveta Makovetska, Oleh Shablykin, Dmytro Lesyk, Galeb Al-Maali, Rodion Korzh, Iryna V. Sadkova and Pavel K. Mykhailiuk\*

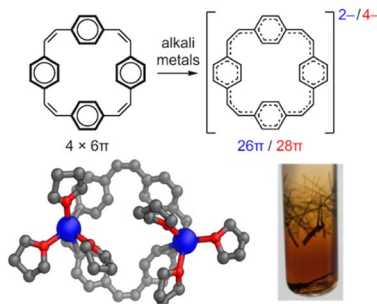
14100



### A single phosphorylation mechanism in early metabolism – the case of phosphoenolpyruvate

Joris Zimmermann, Robert J. Mayer and Joseph Moran\*

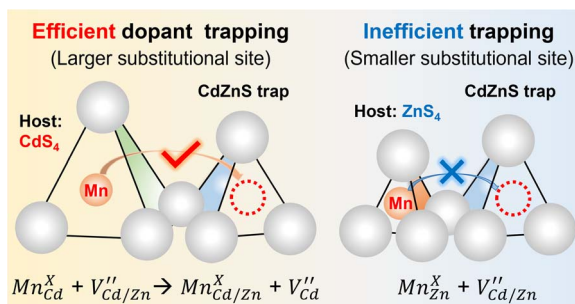
14109



### Crystallographic evidence for global aromaticity in the di-anion and tetra-anion of a cyclophane hydrocarbon

Wojciech Stawski, Yikun Zhu, Zheng Wei, Marina A. Petrukhina\* and Harry L. Anderson\*

14115



### Inserting an "atomic trap" for directional dopant migration in core/multi-shell quantum dots

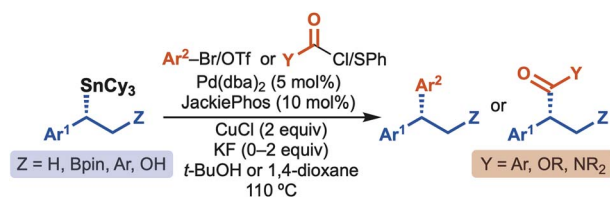
Chun Chu, Elan Hofman, Chengpeng Gao, Shuya Li, Hanjie Lin, Walker MacSwain, John M. Franck, Robert W. Meulenber, Arindam Chakraborty and Weiwei Zheng\*



14124

### A general approach to stereospecific Pd-catalyzed cross-coupling reactions of benzylic stereocenters

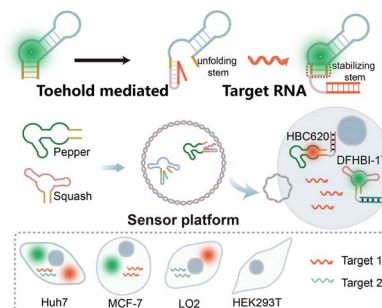
Meruyert Binayeva, Xinghua Ma,  
Pejman Ghaemimohammadi and Mark R. Biscoe\*



14131

### A universal orthogonal imaging platform for living-cell RNA detection using fluorogenic RNA aptamers

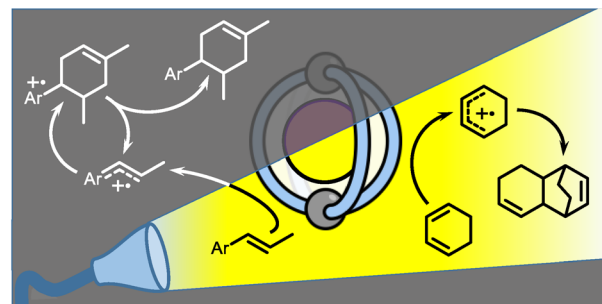
Peng Yin, Mingmin Ge, Shiyi Xie, Li Zhang, Shi Kuang\*  
and Zhou Nie\*



14140

### Exo-cage catalysis and initiation derived from photo-activating host-guest encapsulation

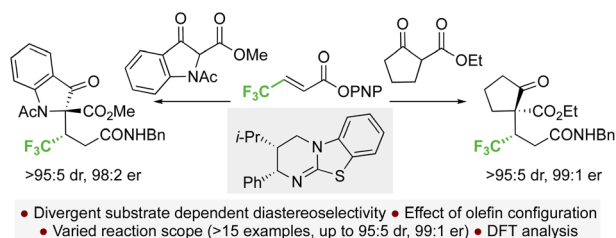
Rebecca L. Spicer, Helen M. O'Connor, Yael Ben-Tal,  
Hang Zhou, Patrick J. Boaler, Fraser C. Milne, Euan  
K. Brechin,\* Guy. C. Lloyd-Jones\* and Paul J. Lusby\*



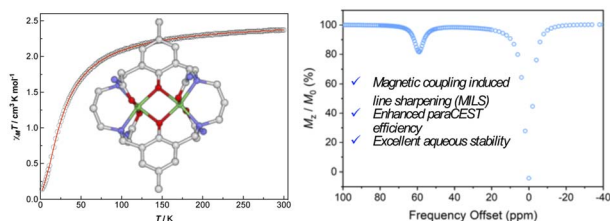
14146

### Understanding divergent substrate stereoselectivity in the isothiurea-catalysed conjugate addition of cyclic $\alpha$ -substituted $\beta$ -ketoesters to $\alpha,\beta$ -unsaturated aryl esters

Ding Yuan, Alister S. Goodfellow, Kevin Kasten,  
Zhuan Duan, Tengfei Kang, David B. Cordes, Aidan  
P. McKay, Michael Bühl,\* Gregory R. Boyce\* and Andrew  
D. Smith\*



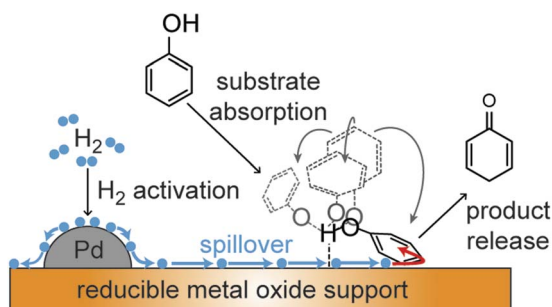
14157



### Improving the potential of paraCEST through magnetic-coupling induced line sharpening

Xin Guo, Lei Zhang, Jiesheng Hu, Balázs Szilágyi, Meng Yu,\* Shizhen Chen,\* Gyula Tircsó, Xin Zhou and Jun Tao\*

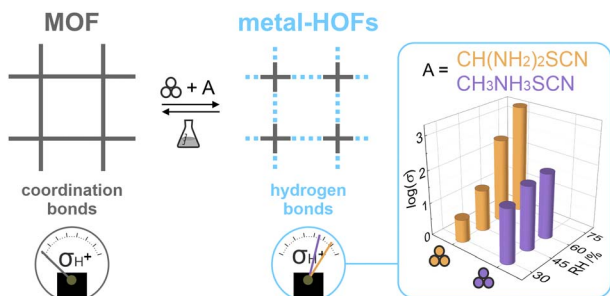
14166



### Hydrogen spillover and substrate–support hydrogen bonding mediate hydrogenation of phenol catalyzed by palladium on reducible metal oxides

Yeongseo An, Puranjan Chatterjee, Pranjali Naik, Sayak Banerjee, Wenyu Huang, Igor I. Slowing and Vincenzo Venditti\*

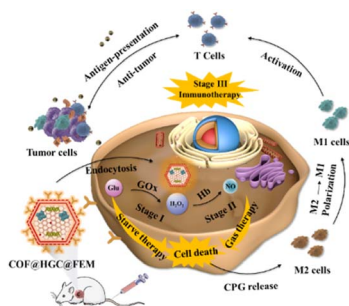
14176



### From non-conductive MOF to proton-conducting metal-HOFs: a new class of reversible transformations induced by solvent-free mechanochemistry

Magdalena Lupa-Myszkowska, Marcin Oszajka and Dariusz Matoga\*

14182



### An erythrocyte membrane-camouflaged fluorescent covalent organic framework for starving/nitric oxide immunotherapy of triple-negative breast cancer

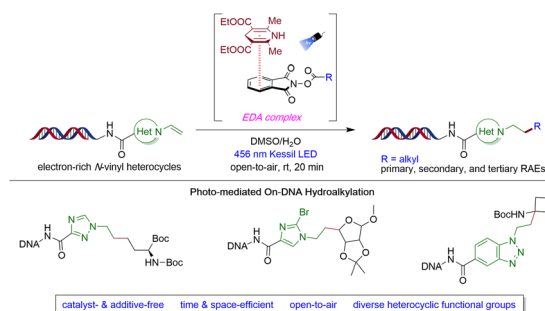
Fang Yuan, Cuiling Zhang,\* Xianzhu Luo, Shasha Cheng, Yingxin Zhu and Yuezhong Xian\*



14193

### On-DNA hydroalkylation of *N*-vinyl heterocycles via photoinduced EDA-complex activation

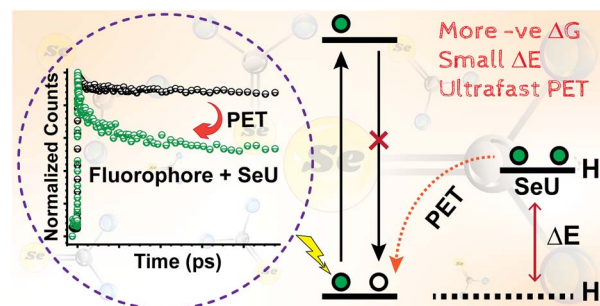
Mohammed Sharique, Bianca Matsuo, Albert Granados, Saegun Kim, Mahwish Arshad, Hyunjung Oh, Victoria E. Wu, Minxue Huang, Adam Csakai, Lisa A. Marcaurelle and Gary A. Molander\*



14200

### Critical assessment of selenourea as an efficient small molecule fluorescence quenching probe to monitor protein dynamics

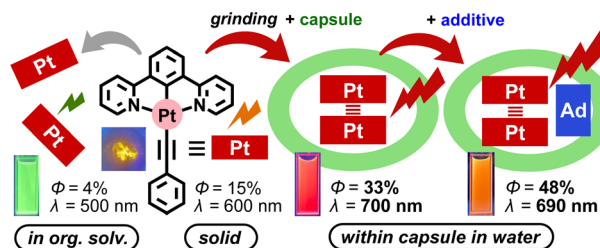
Subhrakant Jena, Kiran Devi Tulsian, Rudhi Ranjan Sahoo, Saiprakash Rout, Akshay Kumar Sahu and Himansu S. Biswal\*



14211

### Solution-state mechanochromic luminescence of Pt(II)-complexes displayed within micellar aromatic capsules

Yoshihisa Hashimoto, Yuri Katagiri, Yuya Tanaka\* and Michito Yoshizawa\*

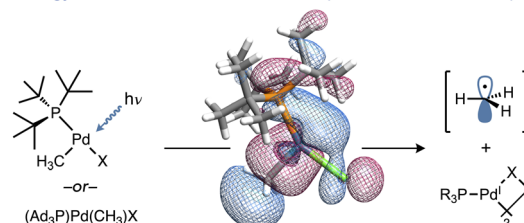


14217

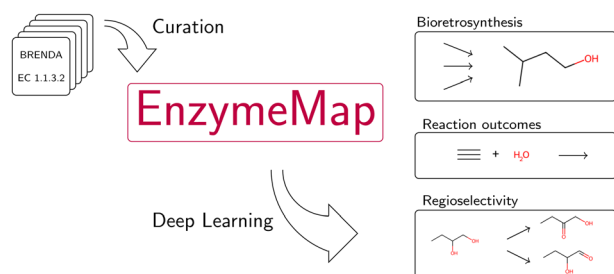
### Visible light-induced palladium–carbon bond weakening in catalytically relevant T-shaped complexes

Peter M. Waddell, Lei Tian, Anthony R. Scavuzzo, Lalu Venigalla, Gregory D. Scholes and Brad P. Carrow\*

low energy d-σ\* transition · redirects ubiquitous Pd(II) into SET pathways



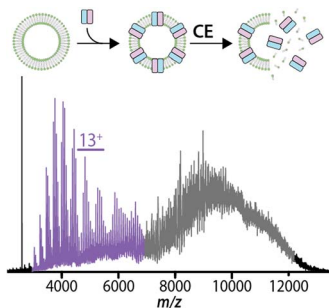
14229



### EnzymeMap: curation, validation and data-driven prediction of enzymatic reactions

Esther Heid,<sup>\*</sup> Daniel Probst, William H. Green and Georg K. H. Madsen

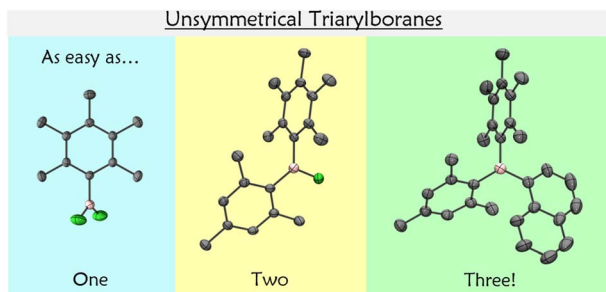
14243



### Native mass spectrometry of proteoliposomes containing integral and peripheral membrane proteins

Yun Zhu, Sangho D. Yun, Tianqi Zhang, Jing-Yuan Chang, Lauren Stover and Arthur Laganowsky<sup>\*</sup>

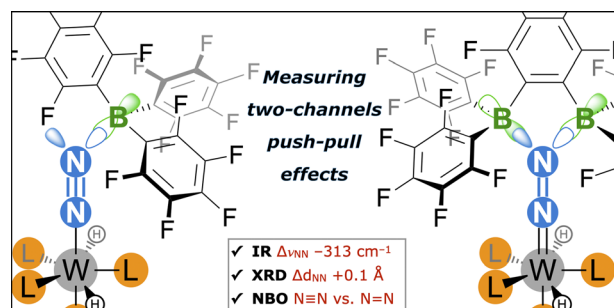
14256



### Rapid, iterative syntheses of unsymmetrical di- and triarylboranes from crystalline aryldifluoroboranes

Douglas Turnbull and Marc-André Légaré<sup>\*</sup>

14262



### An orbitally adapted push-pull template for N<sub>2</sub> activation and reduction to diazene-diide

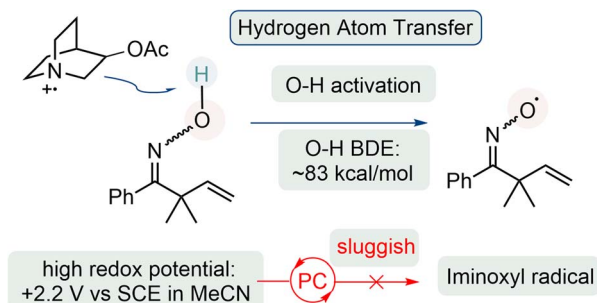
David Specklin, Marie-Christine Boegli, Anaïs Coffinet, Léon Escomel, Laure Vendier, Mary Grellier and Antoine Simonneau<sup>\*</sup>



14271

### O–H bond activation of $\beta,\gamma$ -unsaturated oximes via hydrogen atom transfer (HAT) and photoredox dual catalysis

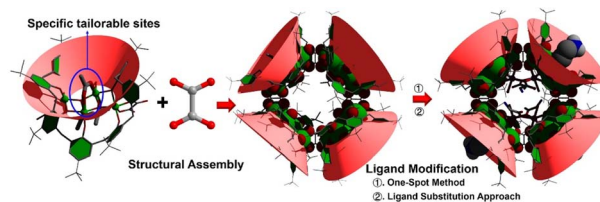
Liang Yi, Chen Zhu, Xiangyu Chen, Huifeng Yue, Tengfei Ji, Yiqiao Ma, Yuanyuan Cao, Rajesh Kancharla and Magnus Rueping\*



14280

### Atomically accurate site-specific ligand tailoring of highly acid- and alkali-resistant Ti(IV)-based metallamacrocycle for enhanced CO<sub>2</sub> photoreduction

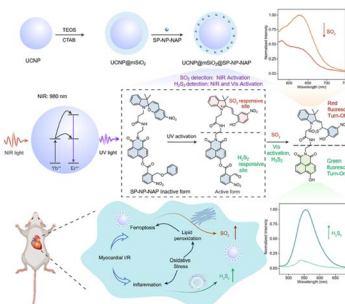
Yi-Qi Tian, Lin-Fang Dai, Wen-Lei Mu, Wei-Dong Yu, Jun Yan\* and Chao Liu\*



14290

### A near-infrared light-activated nanoprobe for simultaneous detection of hydrogen polysulfide and sulfur dioxide in myocardial ischemia–reperfusion injury

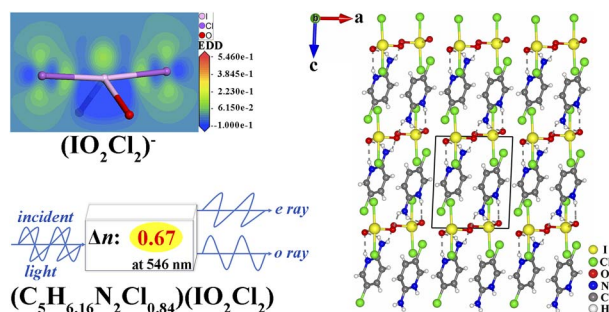
Xianzhu Luo, Cuiling Zhang,\* Chenyang Yue, Yuelin Jiang, Fei Yang and Yuezhong Xian\*



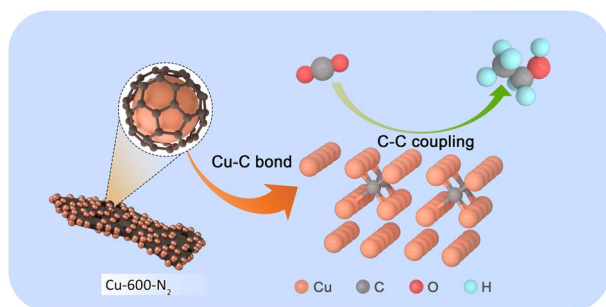
14302

### (C<sub>5</sub>H<sub>6.16</sub>N<sub>2</sub>Cl<sub>0.84</sub>)(IO<sub>2</sub>Cl<sub>2</sub>): a birefringent crystal featuring unprecedented (IO<sub>2</sub>Cl<sub>2</sub>)<sup>-</sup> anions and $\pi$ -conjugated organic cations

Qian-Qian Chen, Chun-Li Hu, Ming-Zhi Zhang and Jiang-Gao Mao\*



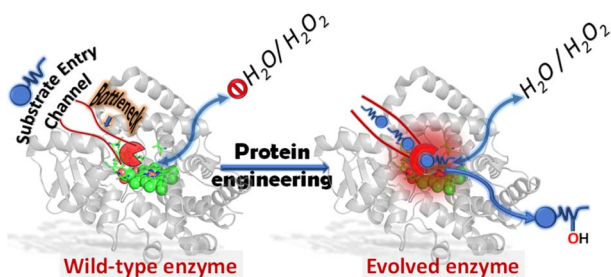
14308



### Optimizing copper nanoparticles with a carbon shell for enhanced electrochemical CO<sub>2</sub> reduction to ethanol

Ting Yao, Wei Xia,\* Shitao Han, Shuaiqiang Jia, Xue Dong, Min Wang, Jiapeng Jiao, Dawei Zhou, Jiahao Yang, Xueqing Xing, Chunjun Chen, Mingyuan He, Haihong Wu\* and Buxing Han\*

14316



### Computationally guided bioengineering of the active site, substrate access pathway, and water channels of thermostable cytochrome P450, CYP175A1, for catalyzing the alkane hydroxylation reaction

Mohd Taher,\* Kshatresh Dutta Dubey\* and Shyamalava Mazumdar\*

