

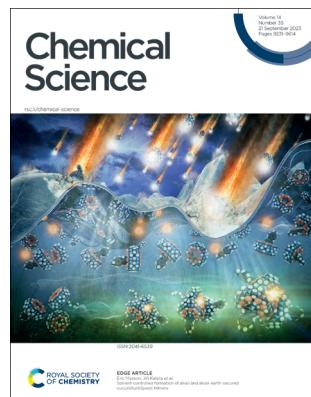
# Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

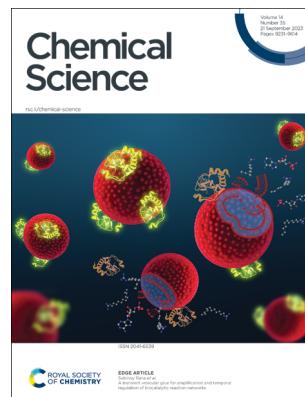
## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(35) 9231–9614 (2023)



### Cover

See Eric Masson, Jiří Kaleta et al., pp. 9258–9266.  
Image reproduced by permission of Tomáš Belloň from *Chem. Sci.*, 2023, 14, 9258.



### Inside cover

See Subinoy Rana et al., pp. 9267–9282. Image reproduced by permission of Subinoy Rana from *Chem. Sci.*, 2023, 14, 9267.

## EDITORIAL

9244

### Highlights from the 56th Bürgenstock Conference on Stereochemistry 2023

Marc Reid\* and Christopher J. Teskey\*

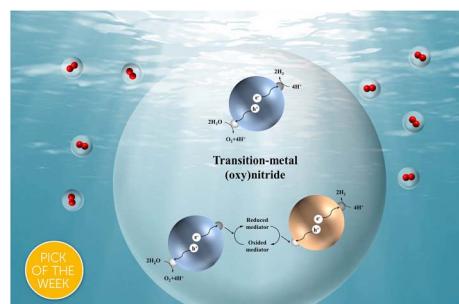


## PERSPECTIVE

9248

### Transition-metal (oxy)nitride photocatalysts for water splitting

Kaihong Chen, Jiadong Xiao, Takashi Hisatomi and Kazunari Domen\*



# Chemical Science

rsc.li/chemical-science

## 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)

## 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 Gabbaï, Texas A&M University  
Subi George, JNCASR  
Ryan Gilmore, 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 Mérida  
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, DIPC-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, MPI-CI  
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, Janseen Research/J&J  
R. Klausen, Johns Hopkins University  
Y. Krishnam, 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, DIPC-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. Reisner, 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  
H. Shafaat, UCLA  
T. Snaddon, Indiana University  
M. Solà, University of Girona  
G. Soler-llia, 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, NCNST  
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. Zarbin, UPFR  
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

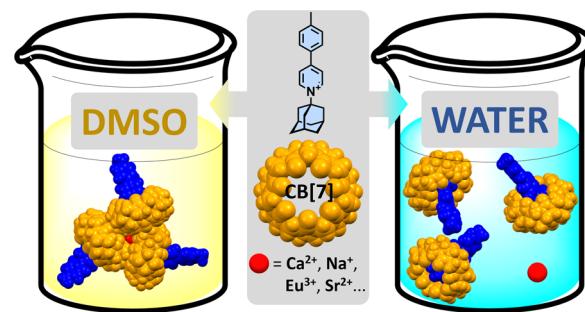


## EDGE ARTICLES

9258

**Solvent-controlled formation of alkali and alkali-earth-secured cucurbituril/guest trimers**

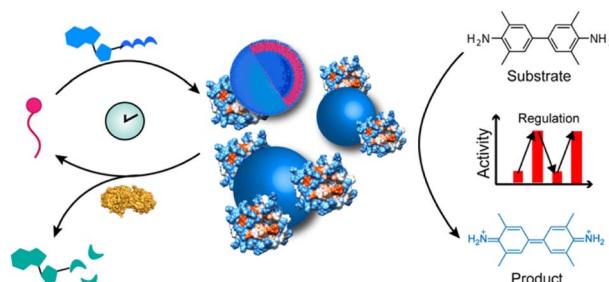
Doroteja Lončarić, Fahimeh Movahedifar, Jakub Radek Štoček, Martin Dračinský, Josef Cvačka, Shanshan Guan, Benjamin J. Bythell, Ivana Císařová, Eric Masson\* and Jiří Kaleta\*



9267

**A transient vesicular glue for amplification and temporal regulation of biocatalytic reaction networks**

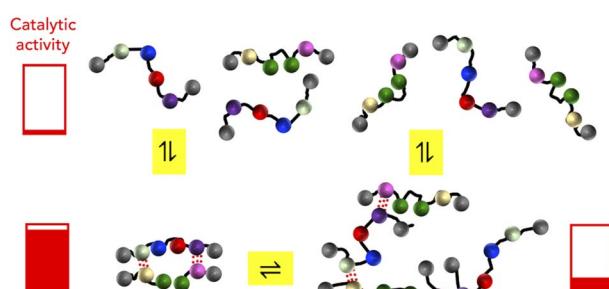
Alisha Kamra, Sourav Das, Preeti Bhatt, Manju Solra, Tanmoy Maity and Subinoy Rana\*



9283

**Dynamic self-assembly of supramolecular catalysts from precision macromolecules**

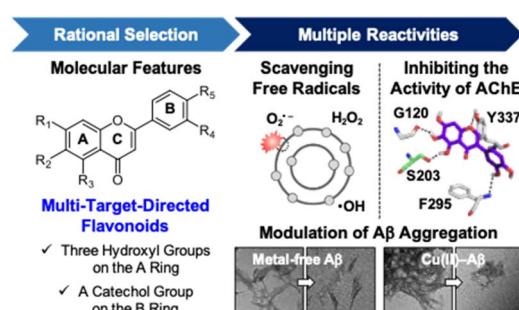
Qian Qin, Jie Li, David Dellemme, Mathieu Fossépré, Gabriella Barozzino-Consiglio, Imane Nekka, Adrian Boborodea, Antony E. Fernandes, Karine Glinel, Mathieu Surin\* and Alain M. Jonas\*



9293

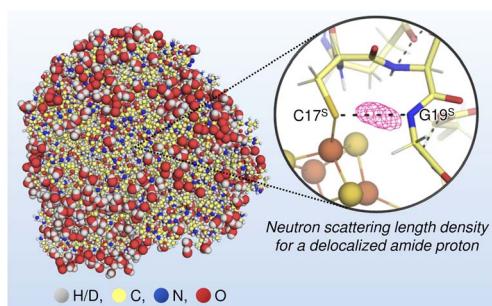
**Designing multi-target-directed flavonoids: a strategic approach to Alzheimer's disease**

Seongmin Park, Mingeun Kim, Yuxi Lin, Mannkyu Hong, Geewoo Nam, Adam Mieczkowski, József Kardos, Young-Ho Lee\* and Mi Hee Lim\*



## EDGE ARTICLES

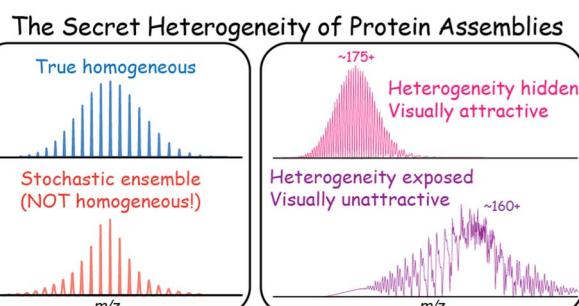
9306



**New insights into the oxidation process from neutron and X-ray crystal structures of an  $O_2^-$ -sensitive [NiFe]-hydrogenase**

Takeshi Hiromoto, Koji Nishikawa, Seiya Inoue, Hideaki Ogata, Yuta Hori, Katsuhiro Kusaka, Yu Hirano, Kazuo Kurihara, Yasuteru Shigeta, Taro Tamada\* and Yoshiaki Higuchi\*

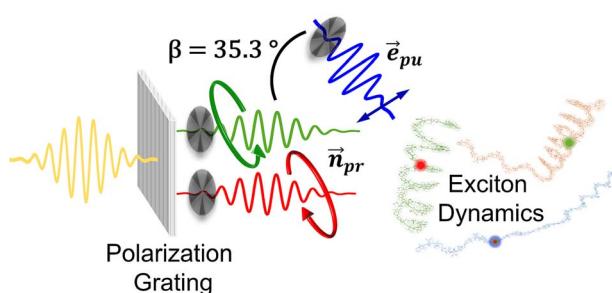
9316



**Stochastic assembly of biomacromolecular complexes: impact and implications on charge interpretation in native mass spectrometry**

Victor Yin, Paul W. A. Devine, Janet C. Saunders, Arjan Barendregt, Fiona Cusdin, Alexandra Ristani, Alistair Hines, Sam Shepherd, Marcin Dembek, Claire L. Dobson, Joost Snijder, Nicholas J. Bond and Albert J. R. Heck\*

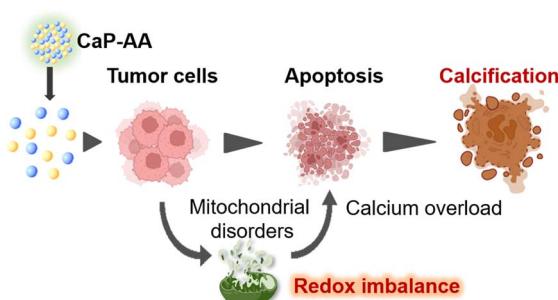
9328



**Time-resolved circular dichroism of excitonic systems: theory and experiment on an exemplary squaraine polymer**

Lea Ress, Pavel Malý, Jann B. Landgraf, Dominik Lindorfer, Michael Hofer, Joshua Selby, Christoph Lambert, Thomas Renger\* and Tobias Brixner\*

9350



**Responsive calcium-derived nanoassemblies induce mitochondrial disorder to promote tumor calcification**

Yan Zhao, Xinquan Yu, Weiheng Kong, Rong-Mei Kong, Ensheng Zhang, Lian Xia, Jing Zhang, Fengli Qu\* and Weihong Tan

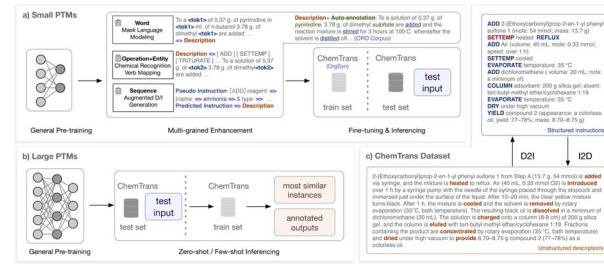


## EDGE ARTICLES

9360

## Transcription between human-readable synthetic descriptions and machine-executable instructions: an application of the latest pre-training technology

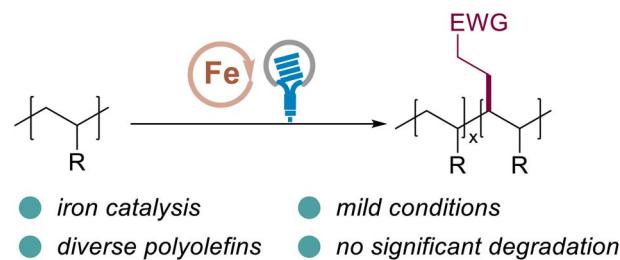
Zheni Zeng, Yi-Chen Nie, Ning Ding, Qian-Jun Ding, Wei-Ting Ye, Cheng Yang, Maosong Sun, Weinan E, Rong Zhu\* and Zhiyuan Liu\*



9374

## Photoinduced iron-catalyzed C–H alkylation of polyolefins

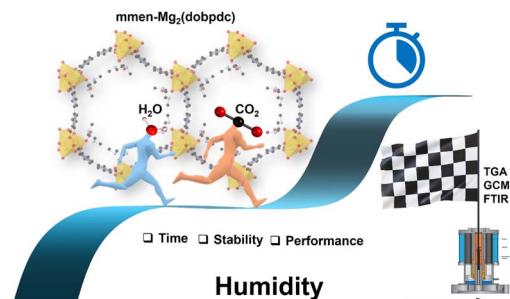
Zongnan Zhang, Yanfeng Zhang and Rong Zeng\*



9380

## Suitability of a diamine functionalized metal–organic framework for direct air capture

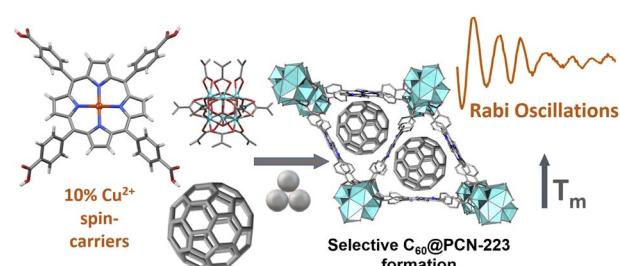
Saptasree Bose, Debabrata Sengupta, Christos D. Malliakas, Karam B. Idrees, Haomiao Xie, Xiaoliang Wang, Michael L. Barsoum, Nathaniel M. Barker, Vinayak P. Dravid, Timur Islamoglu and Omar K. Farha\*



9389

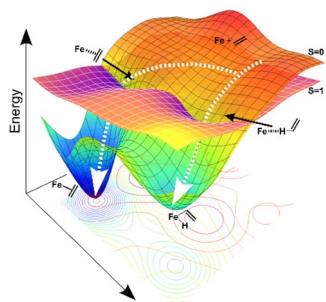
## Improving the molecular spin qubit performance in zirconium MOF composites by mechanochemical dilution and fullerene encapsulation

Lucija Vujević, Bahar Karadeniz,\* Nikola Cindro, Andraž Krajnc, Gregor Mali, Matjaž Mazaj, Stanislav M. Avdoshenko, Alexey A. Popov, Dijana Žilić,\* Krinoslav Užarević\* and Marina Kveder\*



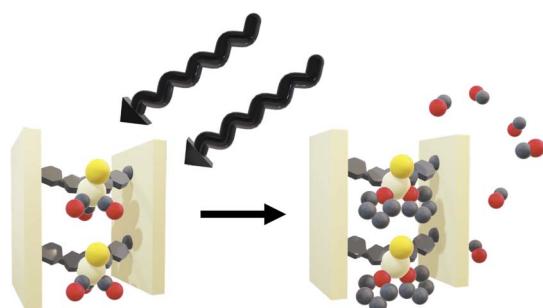
## EDGE ARTICLES

9400


**Dynamic-dependent selectivity in a bisphosphine iron spin crossover C–H insertion/π-coordination reaction**

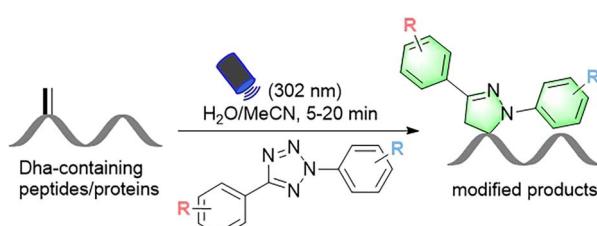
Michael T. Davenport, Justin K. Kirkland and Daniel H. Ess\*

9409


**Studying manganese carbonyl photochemistry in a permanently porous metal–organic framework**

Rosemary J. Young, Michael T. Huxley, Lingjun Wu, Jack Hart, James O'Shea, Christian J. Doonan, Neil R. Champness\* and Christopher J. Sumby\*

9418

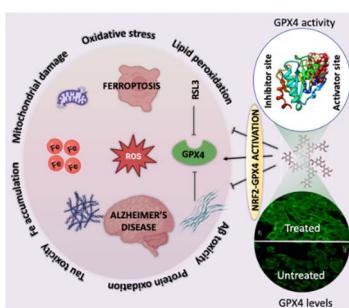


- ✓ Fast reaction kinetics
- ✓ Catalyst-free, mild reaction conditions
- ✓ Photo-controlled
- ✓ Fluorescence "turn on"

**Light-initiated 1,3-dipolar cycloaddition between dehydroalanines and tetrazoles: application to late-stage peptide and protein modifications**

Mengqian Zhang, Peiyang He and Yanmei Li\*

9427


**A natural polyphenol activates and enhances GPX4 to mitigate amyloid-β induced ferroptosis in Alzheimer's disease**

Prayasee Baruah, Hariharan Moorthy, Madhu Ramesh, Dikshaa Padhi and Thimmaiah Govindaraju\*

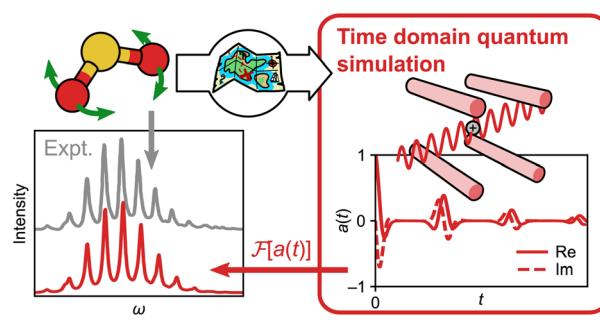


## EDGE ARTICLES

9439

**Predicting molecular vibronic spectra using time-domain analog quantum simulation**

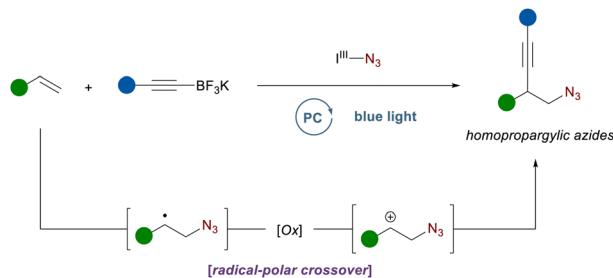
Ryan J. MacDonell, Tomas Navickas, Tim F. Wohlers-Reichel, Christophe H. Valahu, Arjun D. Rao, Maverick J. Millican, Michael A. Currington, Michael J. Biercuk, Ting Rei Tan, Cornelius Hempel\* and Ivan Kassal\*



9452

**Azido-alkynylation of alkenes through radical-polar crossover**

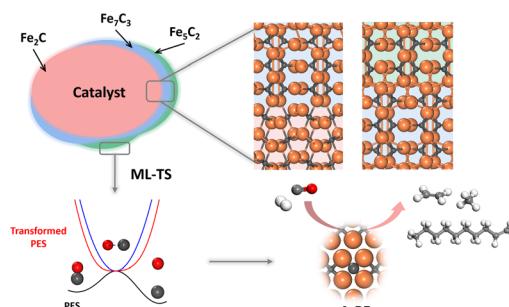
Julien Borrel and Jerome Waser\*



9461

**An optimal Fe–C coordination ensemble for hydrocarbon chain growth: a full Fischer–Tropsch synthesis mechanism from machine learning**

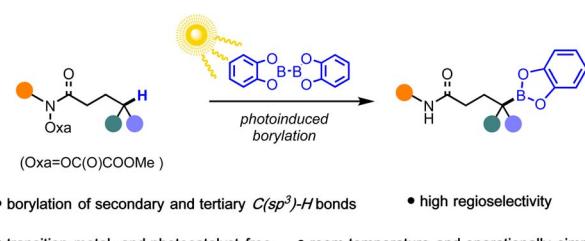
Qian-Yu Liu, Dongxiao Chen, Cheng Shang\* and Zhi-Pan Liu\*



9476

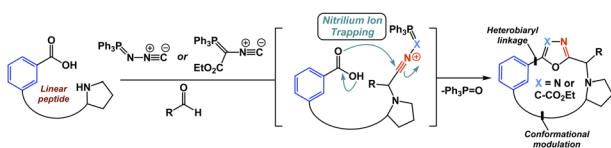
**Metal-free, photoinduced remote C(sp<sup>3</sup>)–H borylation**

Jiachen He and Silas P. Cook\*



## EDGE ARTICLES

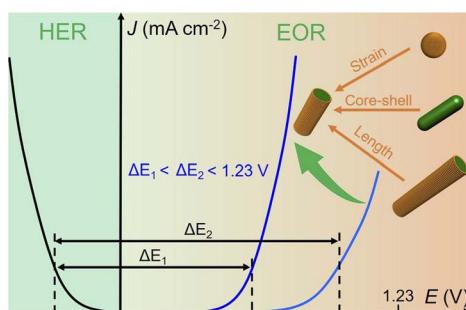
9482



### Nitrilium ion trapping as a strategy to access structurally diverse heterobiaryl-containing peptide macrocycles

Matthew Diamandas, Nicholas W. Heller and Andrei K. Yudin\*

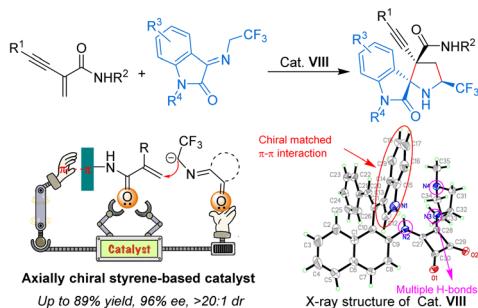
9488



### Length-tunable Pd<sub>2</sub>Sn@Pt core–shell nanorods for enhanced ethanol electrooxidation with concurrent hydrogen production

Tong Li, Qiuxia Wang, Wenjie Zhang, Huaming Li, Yong Wang\* and Junfeng Liu\*

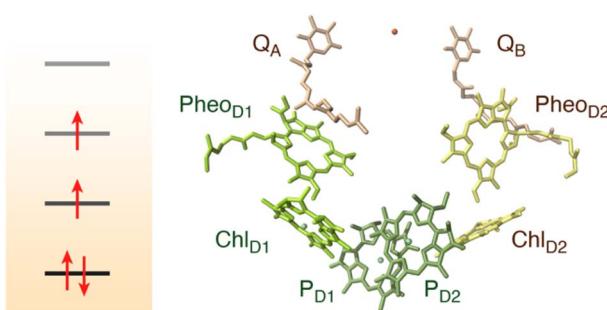
9496



### Axially chiral styrene-based organocatalysts and their application in asymmetric cascade Michael/cyclization reaction

Yu Hao, Zi-Hao Li, Zhi-Gang Ma, Ru-Xin Liu, Rui-Tian Ge, Quan-Zhe Li, Tong-Mei Ding and Shu-Yu Zhang\*

9503



### Triplet states in the reaction center of Photosystem II

Sinjini Bhattacharjee, Frank Neese and Dimitrios A. Pantazis\*



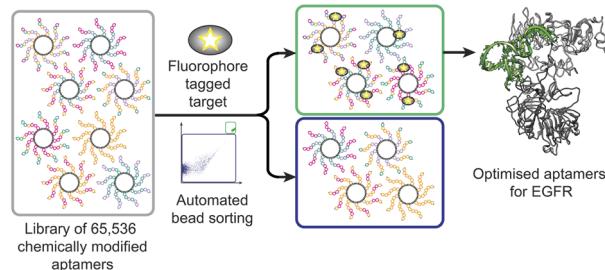
## EDGE ARTICLES

9517

**Selection of optimised ligands by fluorescence-activated bead sorting**

Alexandra R. Paul, Mario Falsaperna, Helen Lavender, Michelle D. Garrett\* and Christopher J. Serpell\*

How and where should aptamers be chemically modified?



9526

**Reductive photoredox transformations of carbonyl derivatives enabled by strongly reducing photosensitizers**

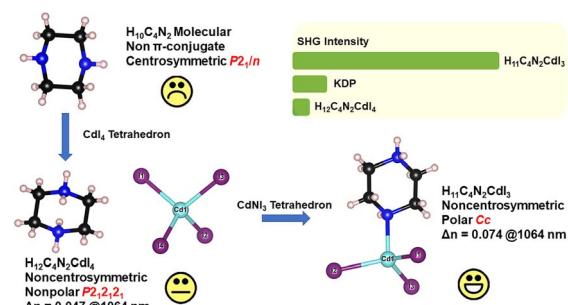
Vinh Q. Dang and Thomas S. Teets\*



9533

**From  $H_{12}C_4N_2CdI_4$  to  $H_{11}C_4N_2CdI_3$ : a highly polarizable  $CdNi_3$  tetrahedron induced a sharp enhancement of second harmonic generation response and birefringence**

Huai-Yu Wu, Chun-Li Hu,\* Miao-Bin Xu, Qian-Qian Chen, Nan Ma, Xiao-Ying Huang, Ke-Zhao Du\* and Jin Chen\*



9543

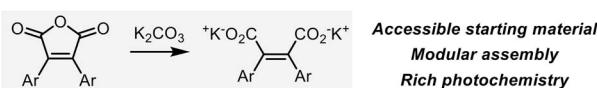
**Porous supramolecular gels produced by reversible self-gelation of ruthenium-based metal–organic polyhedra**

Javier Troyano,\* Fuerkaiti Tayier, Phitchayapha Phattharaphuti, Takuma Aoyama, Kenji Urayama and Shuhei Furukawa\*



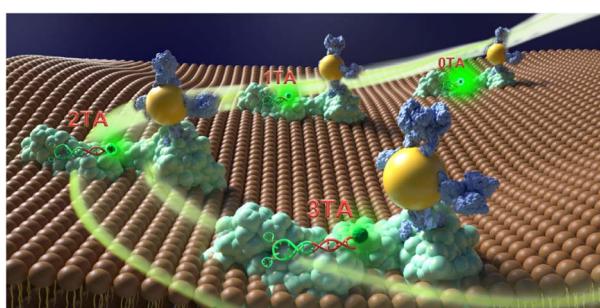
## EDGE ARTICLES

9553

*Pushing the diarylethene photochemistry to water***2,3-Diarylmaleate salts as a versatile class of diarylethenes with a full spectrum of photoactivity in water**

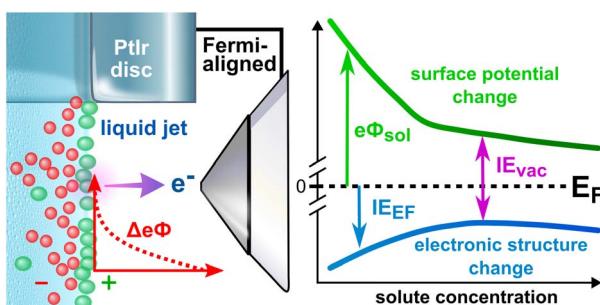
Iumzhana A. Bolotova, Alexander O. Ustyuzhanin, Ekaterina S. Sergeeva, Anna A. Faizdrakhmanova, Yu Hai, Andrey V. Stepanov, Igor A. Ushakov, Konstantin A. Lyssenko, Lei You\* and Andrey G. Lvov\*

9560

**Single-nucleobase resolution of a surface energy transfer nanoruler for *in situ* measurement of aptamer binding at the receptor subunit level in living cells**

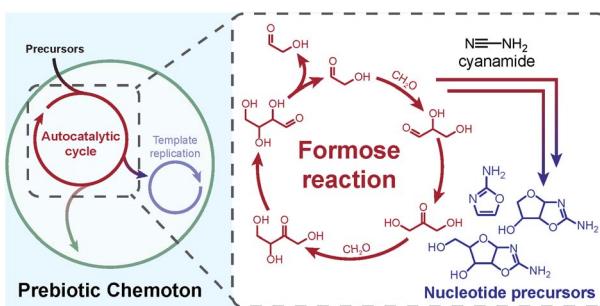
Yu Zhang, Mengke Su, Xingru Fang, Wenwen Huang, Hao Jiang, Qi Li, Nisar Hussain, Mao Ye, Honglin Liu\* and Weihong Tan\*

9574

**How to measure work functions from aqueous solutions**

Michele Pugini, Bruno Credidio, Irina Walter, Sebastian Malerz, Florian Trinter, Dominik Stemmer, Uwe Hergenhahn, Gerard Meijer, Iain Wilkinson, Bernd Winter\* and Stephan Thürmer\*

9589

**Towards a prebiotic chemoton – nucleotide precursor synthesis driven by the autocatalytic formose reaction**

Quoc Phuong Tran, Ruiqin Yi and Albert C. Fahrenbach\*

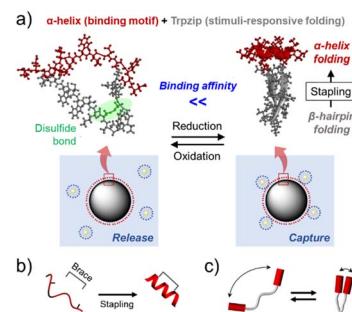


## EDGE ARTICLES

9600

**Modulating the folding and binding of peptides using a stimuli-responsive molecular tweezer**

Sooho Ko, Joo-Young Kim, Jung Yeon Park, You-jin Jung, Min-Jae Choi, Kyeong Sik Jin, Yongju Kim, Yong-beom Lim\* and Woo-jin Jeong\*



## CORRECTIONS

9608

**Correction: Structural tuning of organoruthenium compounds allows oxidative switch to control ER stress pathways and bypass multidrug resistance**

Mun Juinn Chow, Cynthia Licona, Giorgia Pastorin, Georg Mellitzer, Wee Han Ang\* and Christian Gaiddon\*

9610

**Correction: A H<sub>2</sub>O<sub>2</sub> self-sufficient nanoplatform with domino effects for thermal-responsive enhanced chemodynamic therapy**

Shichao Zhang, Changyu Cao, Xinyi Lv, Hanming Dai, Zhihao Zhong, Chen Liang, Wenjun Wang, Wei Huang, Xuejiao Song\* and Xiaochen Dong\*