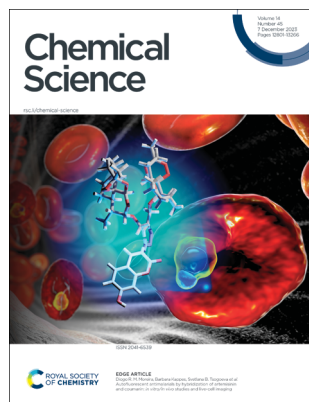


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(45) 12801–13266 (2023)



**Cover**  
See Diogo R. M. Moreira, Barbara Kappes, Svetlana B. Tsogoeva *et al.*, pp. 12941–12952. Image reproduced by permission of Diogo R. M. Moreira and Svetlana B. Tsogoeva from *Chem. Sci.*, 2023, **14**, 12941.



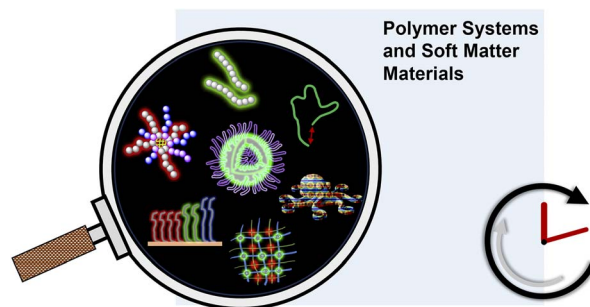
**Inside cover**  
See Tomás Martín *et al.*, pp. 12953–12960. Image reproduced by permission of Manuel Rondelli, Noelia Labrador-García and Juan Carlos Acosta-Hernández from *Chem. Sci.*, 2023, **14**, 12953. Artwork by Manuel Rondelli, Noelia Labrador-García and Juan Carlos Acosta-Hernández.

## REVIEWS

12815

### Fluorescence-readout as a powerful macromolecular characterisation tool

Xingyu Wu and Christopher Barner-Kowollik\*

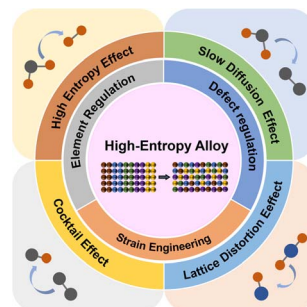


Polymer Systems  
and Soft Matter  
Materials

12850

### Optimization strategies of high-entropy alloys for electrocatalytic applications

Liyuan Xiao, Zhenlu Wang\* and Jingqi Guan\*



# Chemical Science

rsc.li/chemical-science

## Editorial Board

### Editor-in-Chief

Andrew Cooper, University of Liverpool

### Associate Editors

Vincent Artero, CEA-Grenoble  
Luis M. Campos, Columbia University  
Michelle Chang, University of California, Berkeley  
Lin X. Chen, Northwestern University  
Graeme Day, University of Southampton  
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Mircea Dincă, MIT

François Gabbai, Texas A&M University  
Subi George, JNCASR  
Ryan Gilmour, WWU Münster  
Jinlong Gong, Tianjin University  
Stephen Goldup, University of Birmingham  
Zaiping Guo, University of Adelaide  
Christopher A. Hunter, University of Cambridge  
Malika Jefferies-EL, Boston University  
Ning Jiao, Peking University  
Tanja Junkers, Monash University

Hemamala Karunadasa, Stanford University  
Maja Köhn, University of Freiburg  
Yi-Tao Long, Nanjing University  
Gabriel Merino, CINVESTAV Merida  
James K. McCusker, Michigan State University  
Thomas Meade, Northwestern University  
Paolo Melchiorre, University of Bologna  
Carsten Schultz, Oregon Health & Science University  
Dmitri Talapin, The University of Chicago  
Toshiharu Teranishi, Kyoto University  
Andrei Yudin, University of Toronto

## Advisory Board

D. Adams, University of Glasgow  
A. Ajayaghosh, NIIST  
R. Amaro, UC San Diego  
A. Anastasaki, ETH Zürich  
U.-P. Apfel, Ruhr-University Bochum  
K. Asmis, Leipzig University  
X. Bao, DICP-CAS  
Z. Bao, Stanford University  
D. N. Beratan, Duke University  
G. Bernardes, University of Cambridge  
F. Biedermann, KIT  
D. Blackmond, Scripps Research Institute  
E. Blasco, Heidelberg University  
J. Bode, ETH Zurich  
J. S. Brodbelt, UT Austin  
C. Chang, UC Berkeley  
C.-M. Che, University of Hong Kong  
J. Chen, Nankai University  
M. Cohen, OHSU  
C. Coley, MIT  
J. Cornella, MPIC  
L. Cronin, University of Glasgow  
J. Crowley, University of Otago  
C. C. Cummins, MIT  
V. Däschlein-Gessner, Ruhr University Bochum  
M. Delbianco, MPICI  
J. Dempsey, UNC Chapel Hill  
W. Dichtel, Northwestern University  
K. Domen, University of Tokyo  
H. Duan, Tsinghua University  
X. Feng, TU Dresden  
B. Feringa, University of Groningen  
J. Figueroa, UC San Diego  
N. Frank, University of Nevada  
M. Freitag, Newcastle University  
S. Gao, Peking University  
J. Gassensmith, UT Dallas  
G. Gasser, PSL University  
E. Gibson, Newcastle University  
R. Gilliard, Jr., MIT  
F. Glorius, WWU Münster  
L. González, University of Vienna  
D. Graham, University of Strathclyde  
V. Grassian, UC San Diego  
A. Grimaud, Collège de France/CNRS  
T. Gulder, Leipzig University  
W. 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. Zharbin, UFPR  
L. Zhang, ECNU  
T. Zhang, TIPCC-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/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](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)

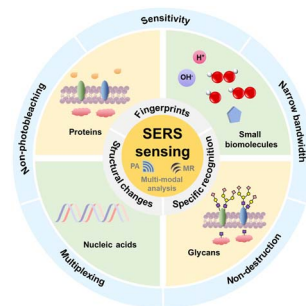


## REVIEWS

12869

**Surface-enhanced Raman scattering sensing for detection and mapping of key cellular biomarkers**

Yuanjiao Yang, Shan Wu, Yunlong Chen\* and Huangxian Ju\*

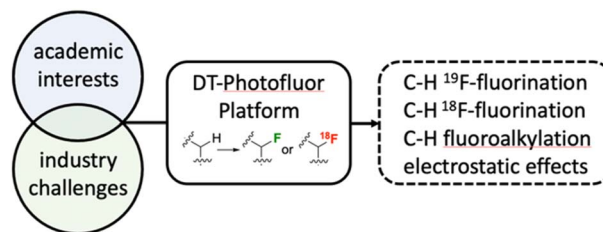


## PERSPECTIVES

12883

**Development and application of decatungstate catalyzed C–H <sup>18</sup>F- and <sup>19</sup>F-fluorination, fluoroalkylation and beyond**

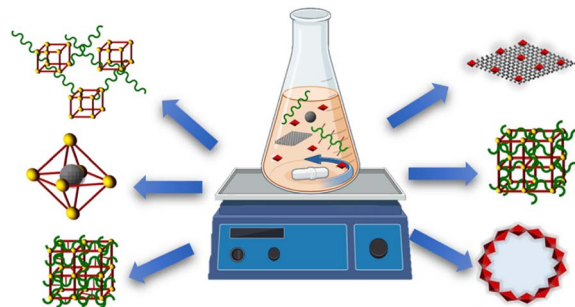
Zheliang Yuan\* and Robert Britton\*



12898

**Interfacing metal organic frameworks with polymers or carbon-based materials: from simple to hierarchical porous and nanostructured composites**

Khaled Dassouki, Sanchari Dasgupta, Eddy Dumas and Nathalie Steunou\*



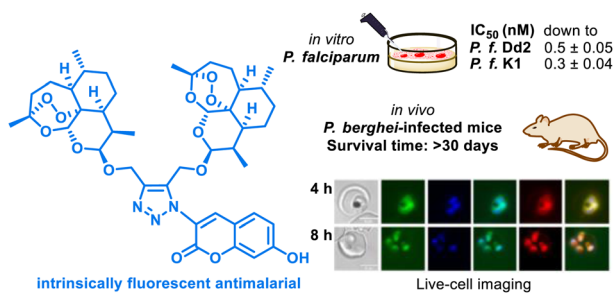
12926

**Sustainable formulation polymers for home, beauty and personal care: challenges and opportunities**

Christina A. R. Picken, Orla Buensoz, Paul D. Price, Christopher Fidge, Laurie Points and Michael P. Shaver\*



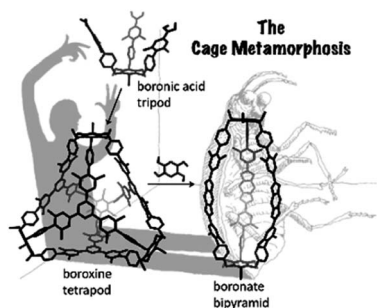
12941



### Autofluorescent antimalarials by hybridization of artemisinin and coumarin: *in vitro/in vivo* studies and live-cell imaging

Lars Herrmann, Maria Leidenberger, Adrielle Sacramento de Morais, Christina Mai, Aysun Çapci, Mariana da Cruz Borges Silva, Fabian Plass, Axel Kahnt, Diogo R. M. Moreira,\* Barbara Kappes\* and Svetlana B. Tsogoeva\*

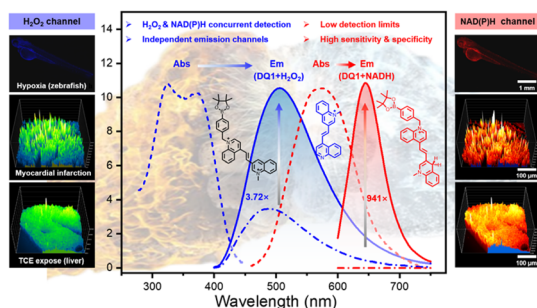
12953



### Conformational control enables boroxine-to-boronate cage metamorphosis

Manuel Rondelli, Samuel Delgado-Hernández, Antonio H. Daranas and Tomás Martín\*

12961



### A dual-responsive ratiometric indicator designed for *in vivo* monitoring of oxidative stress and antioxidant capacity

Majun Yang, Weida Zhu, Yilin Lv, Bin Jiang, Chenxia Jiang, Xiaobo Zhou, Guo Li, Yuling Qin, Qi Wang,\* Ziwei Chen\* and Li Wu\*

12973



### Identification of non-conventional small molecule degraders and stabilizers of squalene synthase

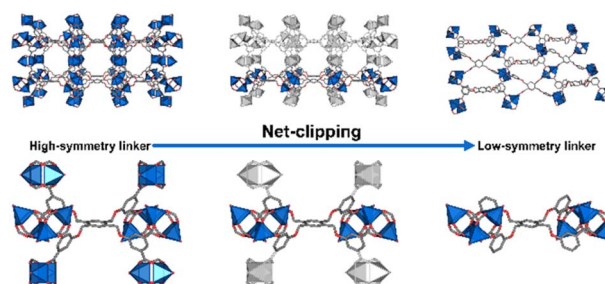
Joseph G. F. Hoock, Cecilia Rossetti, Mesut Bilgin, Laura Depta, Kasper Enemark-Rasmussen, John C. Christianson and Luca Laraia\*



12984

## Net-clipping as a top-down approach for the prediction of topologies of MOFs built from reduced-symmetry linkers

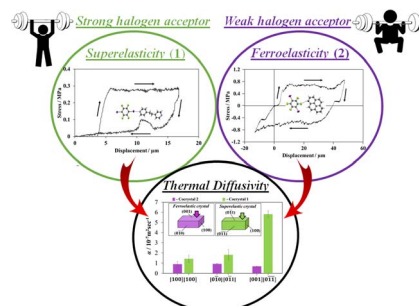
Borja Ortín-Rubio, Jaume Rostoll-Berenguer, Carlos Vila, Davide M. Proserpio, Vincent Guillerm, Judith Juanhuix, Inhar Imaz\* and Daniel Maspoch\*



12995

## A role of intermolecular interaction modulating thermal diffusivity in organosuperelastic and organoferroelastic cocrystals

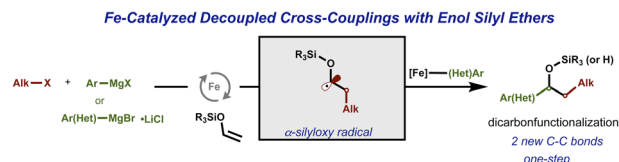
Subham Ranjan, Ryota Morioka, Meguya Ryu, Junko Morikawa\* and Satoshi Takamizawa\*



13007

## Expanding the chemical space of enol silyl ethers: catalytic dicarbofunctionalization enabled by iron catalysis

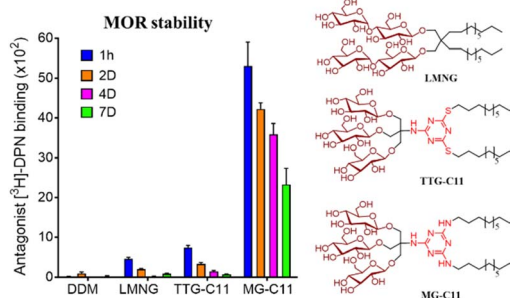
Dinabandhu Sar, Shuai Yin, Jacob Grygus, Ángel Rentería-Gómez, Melanie Garcia and Osvaldo Gutierrez\*



13014

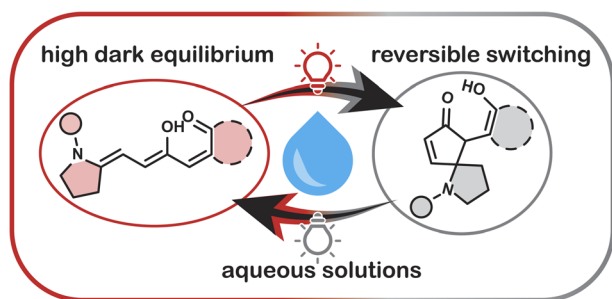
## Melamine-cored glucosides for membrane protein solubilization and stabilization: importance of water-mediated intermolecular hydrogen bonding in detergent performance

Lubna Ghani, Seonghoon Kim, Muhammad Ehsan, Baoliang Lan, Ida H. Poulsen, Chandra Dev, Satoshi Katsube, Bernadette Byrne, Lan Guan, Claus J. Loland, Xiangyu Liu,\* Wonpil Im\* and Pil Seok Chae\*





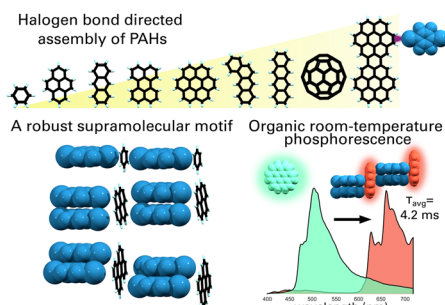
13025



### Tethered together: DASA design towards aqueous compatibility

Julie A. Peterson, Natalia M. Neris and Javier Read de Alaniz\*

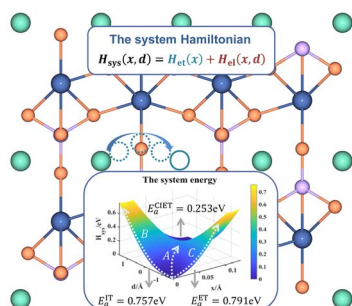
13031



### Halogen bonding with carbon: directional assembly of non-derivatised aromatic carbon systems into robust supramolecular ladder architectures

Jogirdas Vainauskas, Tristan H. Borchers, Mihails Arhangelis, Laura J. McCormick McPherson, Toni S. Spilfogel, Ehsan Hamzehpoor, Filip Topić, Simon J. Coles, Dmytro F. Perepichka, Christopher J. Barrett and Tomislav Friščić\*

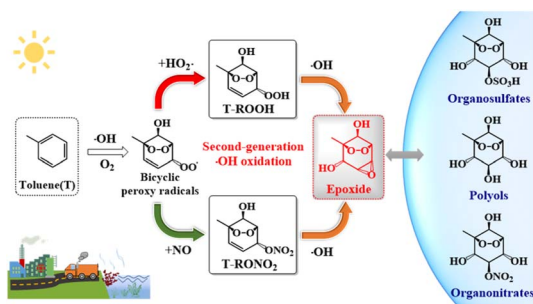
13042



### The decisive role of electrostatic interactions in transport mode and phase segregation of lithium ions in LiFePO<sub>4</sub>

Xiaoxiao Wang, Jun Huang,\* Yuwen Liu and Shengli Chen\*

13050



### An overlooked oxidation mechanism of toluene: computational predictions and experimental validations

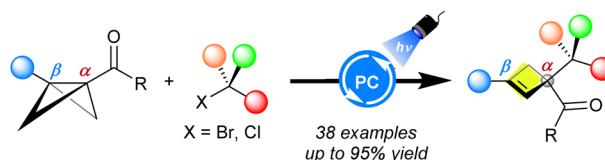
Zihao Fu, Fangfang Ma, Yuliang Liu, Chao Yan, Dandan Huang, Jingwen Chen, Jonas Elm, Yuanyuan Li, Aijun Ding, Lukas Pichelstorfer, Hong-Bin Xie,\* Wei Nie,\* Joseph S. Francisco\* and Putian Zhou\*



13060

### Photochemical $\alpha$ -selective radical ring-opening reactions of 1,3-disubstituted acyl bicyclobutanes with alkyl halides: modular access to functionalized cyclobutenes

Yuanjiu Xiao, Tong-Tong Xu, Jin-Lan Zhou, Feng Wu, Lei Tang, Ruo-Yi Liu, Wen-Biao Wu\* and Jian-Jun Feng\*

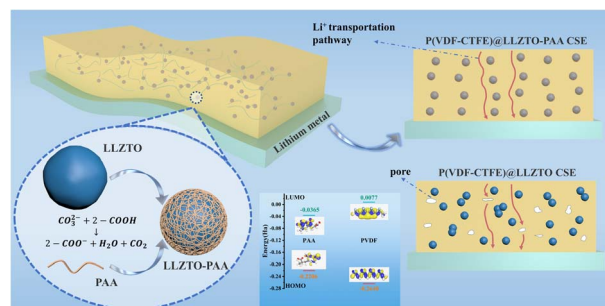


- ✓ Construction of contiguous quaternary all-carbon centers
- ✓ Exclusive  $\alpha$ -selectivity
- ✓ Mild reaction conditions
- ✓ Broad scope and tolerance
- ✓ Modular & concise synthesis

13067

### Surface modification of garnet fillers with a polymeric sacrificial agent enables compatible interfaces of composite solid-state electrolytes

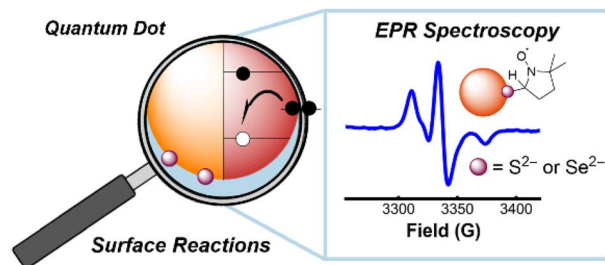
Bin Luo, Jintian Wu, Ming Zhang, Zhihao Zhang, Xingwei Zhang, Zixuan Fang,\* Ziqiang Xu\* and Mengqiang Wu\*



13080

### EPR spin trapping of nucleophilic and radical reactions at colloidal metal chalcogenide quantum dot surfaces

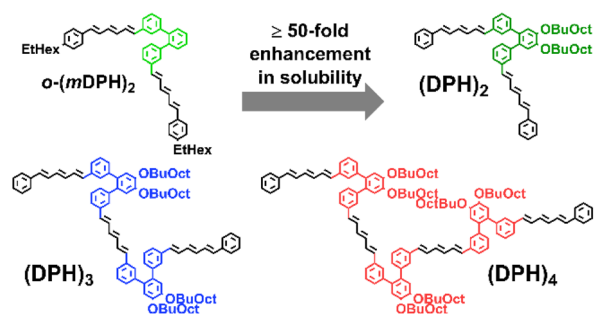
Caroline J. Aschendorf, Mawuli Degbevi, Keaton V. Prather and Emily Y. Tsui\*



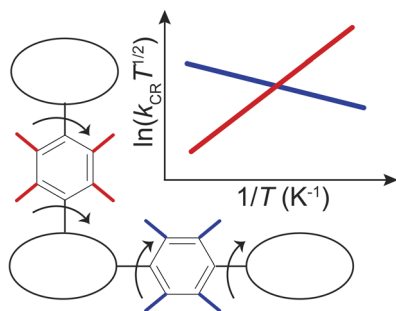
13090

### Synthesis and intramolecular singlet fission properties of *ortho*-phenylene linked oligomers of diphenylhexatriene

Oliver Millington, Ashish Sharma, Stephanie Montanaro, Anastasia Leventis, Simon A. Dowland, Daniel G. Congrave, Cherie-Anne Lee, Akshay Rao\* and Hugo Bronstein\*



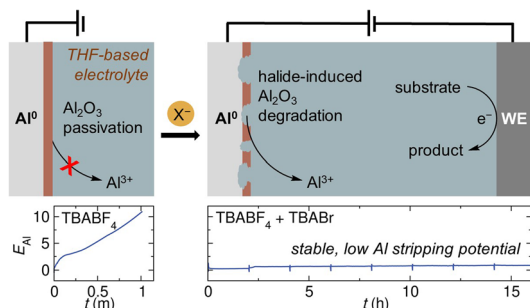
13095



### Anti-Arrhenius behavior of electron transfer reactions in molecular dimers

Neo Lin and Tomoyasu Mani\*

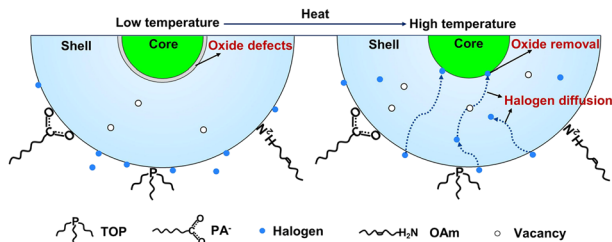
13108



### Enabling Al sacrificial anodes in tetrahydrofuran electrolytes for reductive electroynthesis

Wendy Zhang, Weiyang Guan, Yi Wang, Song Lin and Kimberly A. See\*

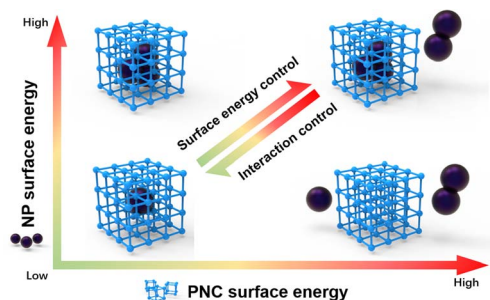
13119



### Interface defects repair of core/shell quantum dots through halide ion penetration

Changwei Yuan, Mengda He, Xinrong Liao, Mingming Liu, Qinggang Zhang, Qun Wan, Zan Qu, Long Kong\* and Liang Li\*

13126



### A highly efficient synthetic strategy for *de novo* NP encapsulation into metal-organic frameworks: enabling further modulated control of catalytic properties

Li Zhou, Yuanyuan An, Jialong Ma, Guoxiu Hao, Zhehui Li, Junchen Chen and Lien-Yang Chou\*

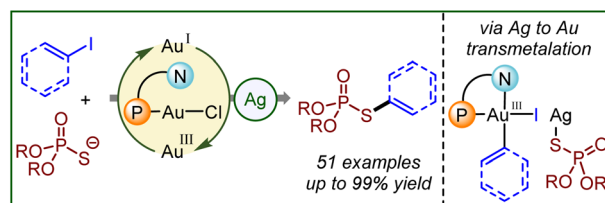




13134

**Gold-catalyzed alkenylation and arylation of phosphorothioates**

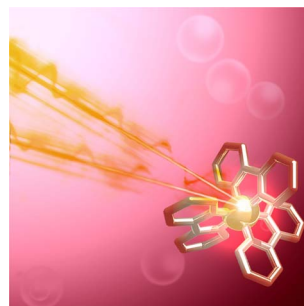
Urvashi, Sampurna Mishra and Nitin T. Patil\*



13140

**Observation of parallel intersystem crossing and charge transfer-state dynamics in  $[\text{Fe}(\text{bpy})_3]^{2+}$  from ultrafast 2D electronic spectroscopy**

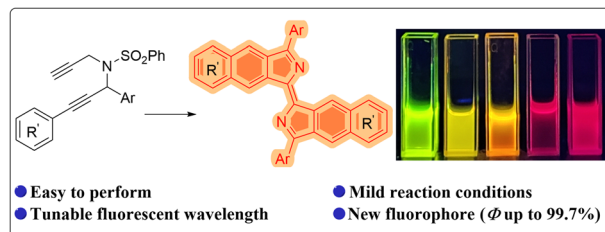
Angela Lee, Minjung Son, Mawuli Deegbey, Matthew D. Woodhouse, Stephanie M. Hart, Hayden F. Beissel, Paul T. Cesana, Elena Jakubikova, James K. McCusker\* and Gabriela S. Schlau-Cohen\*



13151

**Synthesis of a new fluorophore: wavelength-tunable bisbenzo[*f*]isoindolidenes**

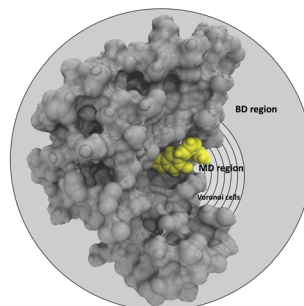
Changqing Ye, Rui Huang, Mong-Feng Chiou, Bo Wang, Daliang Li\* and Hongli Bao\*



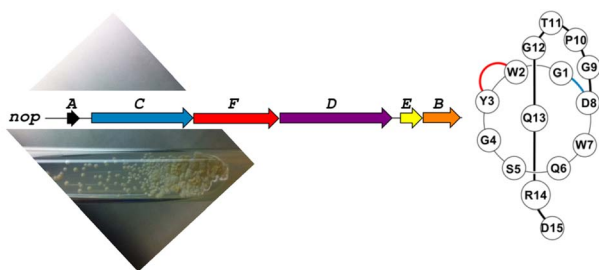
13159

**QMrebind: incorporating quantum mechanical force field reparameterization at the ligand binding site for improved drug-target kinetics through milestone simulations**

Anupam Anand Ojha, Lane William Votapka and Rommie Elizabeth Amaro\*



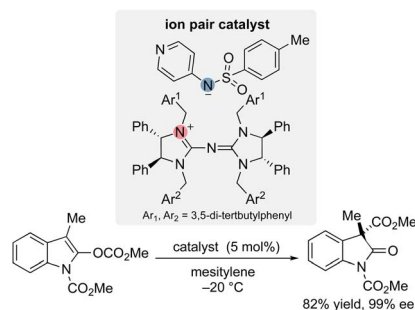
13176



### Bioinformatics-guided discovery of biaryl-linked lasso peptides

Hamada Saad,\* Thomas Majer, Keshab Bhattarai, Sarah Lampe, Dinh T. Nguyen, Markus Kramer, Jan Straetener, Heike Brötz-Oesterhelt, Douglas A. Mitchell and Harald Gross\*

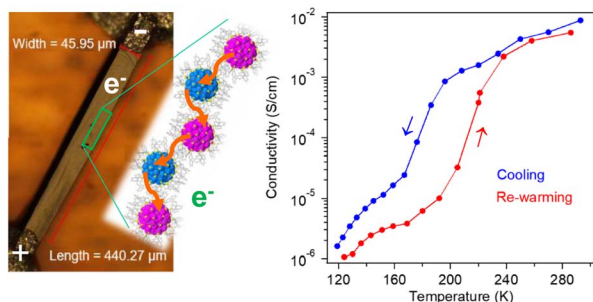
13184



### A chiral pentanidium and pyridinyl-sulphonamide ion pair as an enantioselective organocatalyst for Steglich rearrangement

Ziqi Yang, Chaoran Xu, Xianxian Zhou, Choon Boon Cheong,\* Choon Wee Kee\* and Choon-Hong Tan\*

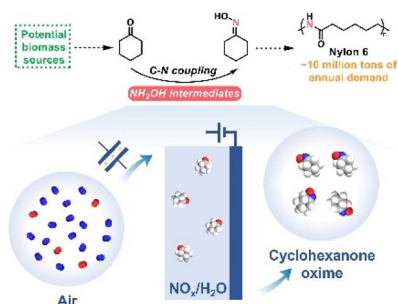
13191



### Electron transport through supercrystals of atomically precise gold nanoclusters: a thermal bi-stability effect

Tatsuya Higaki, Jake C. Russell, Daniel W. Paley, Xavier Roy\* and Rongchao Jin\*

13198



### Integration of plasma and electrocatalysis to synthesize cyclohexanone oxime under ambient conditions using air as a nitrogen source

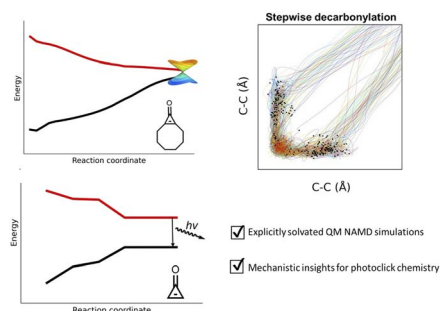
Shunhan Jia, Xingxing Tan, Limin Wu, Xiaodong Ma, Libing Zhang, Jiaqi Feng, Liang Xu, Xinning Song, Qinggong Zhu, Xinchen Kang, Xiaofu Sun\* and Buxing Han\*



13205

### Multiconfigurational photodynamics simulations reveal the mechanism of photodecarbonylations of cyclopropenones in explicit aqueous environments

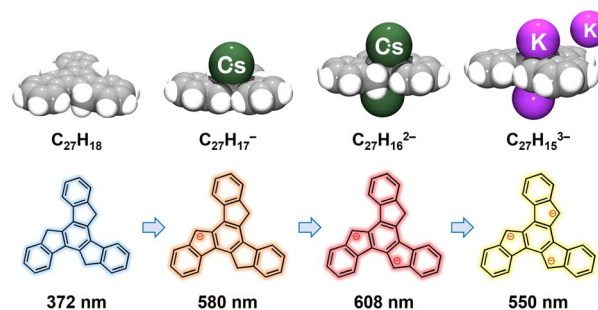
Daniel M. Adrion, Waruni V. Karunaratne and Steven A. Lopez\*



13219

### Stepwise deprotonation of truxene: structures, metal complexation, and charge-dependent optical properties

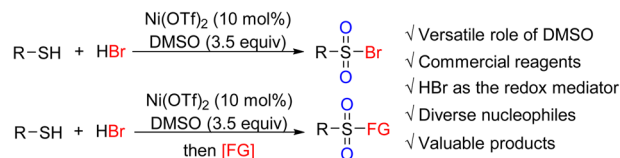
Yumeng Guo, Herdya S. Torchon, Yikun Zhu, Zheng Wei, Zhenyi Zhang, Haixiang Han,\* Marina A. Petrukhina\* and Zheng Zhou\*



13228

### An efficient and mild oxidative approach from thiols to sulfonyl derivatives with DMSO/HBr

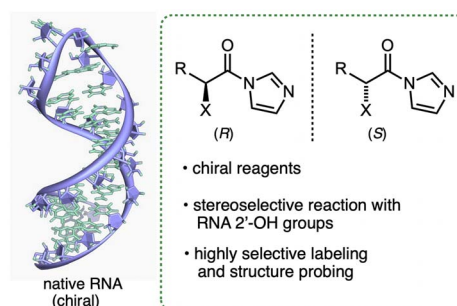
Hongye Wang, Zhaoting Li, Rongheng Dai, Ning Jiao and Song Song\*



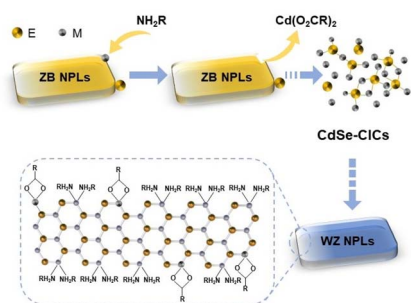
13235

### Stereoselective RNA reaction with chiral 2'-OH acylating agents

Ryuta Shioi, Lu Xiao, Sayantan Chatterjee and Eric T. Kool\*



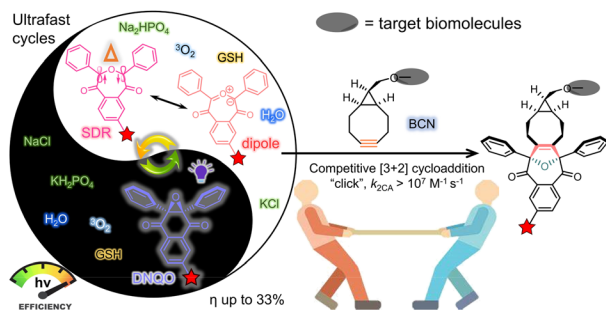
13244



### Covalent inorganic complexes enabled zinc blende to wurtzite phase changes in CdSe nanoplatelets

Xinke Kong, Lin Ru, Junjun Ge, Yalei Deng, Pan-ke Zhang and Yuanyuan Wang\*

13254



### Photoswitchable and long-lived seven-membered cyclic singlet diradicals for the bioorthogonal photoclick reaction

Fuqiang Hu, Cefei Zhang, Zhihao Liu, Xinyu Xie, Xiaohu Zhao, Yanju Luo, Jielin Fu, Baolin Li, Changwei Hu, Zhishan Su\* and Zhipeng Yu\*

