

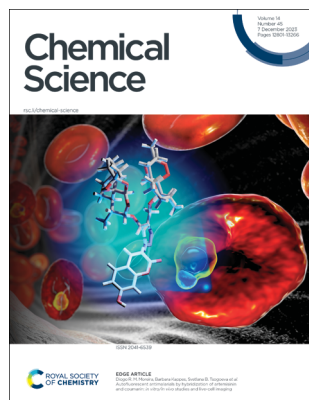
Chemical Science

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(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.



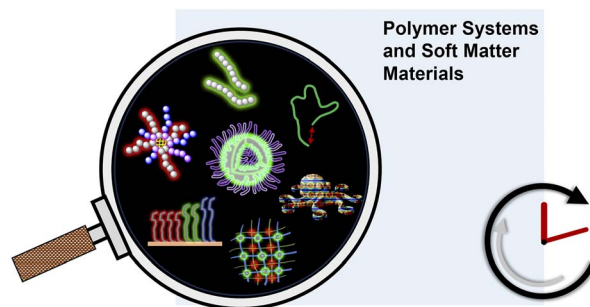
Inside cover
See Tomás Martín *et al.*, pp. 12953–12960. Image reproduced by permission of Manuel Rondelli, Noelia Labrador-García and Juan Carlos Acosta-Hernández from *Chem. Sci.*, 2023, **14**, 12953. Artwork by Manuel Rondelli, Noelia Labrador-García and Juan Carlos Acosta-Hernández.

REVIEWS

12815

Fluorescence-readout as a powerful macromolecular characterisation tool

Xingyu Wu and Christopher Barner-Kowollik*

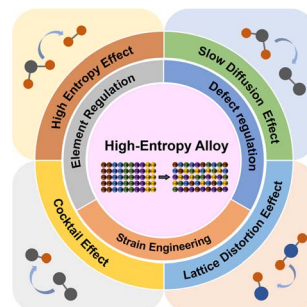


Polymer Systems
and Soft Matter
Materials

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. 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 Copsey

Deputy Editor

Samantha Apps

Senior Editor

James Moore

Scientific Editors

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

Editorial Assistant

Karina Webster

Publishing Assistant

David Bishop

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

For pre-submission queries please contact May Copsey, Executive Editor. E-mail chemicalscience-rsc@rsc.org

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

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

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

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

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

Advertisement sales:

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

For marketing opportunities relating to this journal, contact marketing@rsc.org

Information for Authors

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

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

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

Registered charity number: 207890

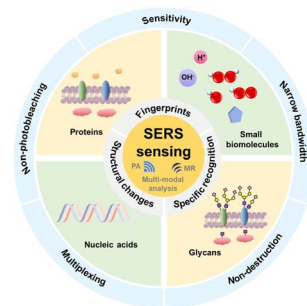


REVIEWS

12869

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

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

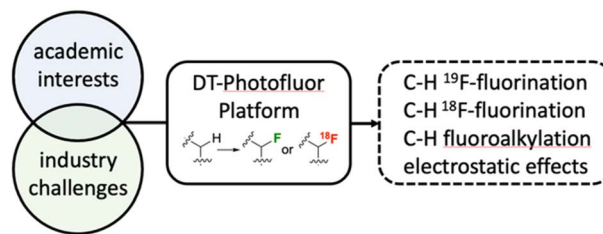


PERSPECTIVES

12883

Development and application of decatungstate catalyzed C–H ¹⁸F- and ¹⁹F-fluorination, fluoroalkylation and beyond

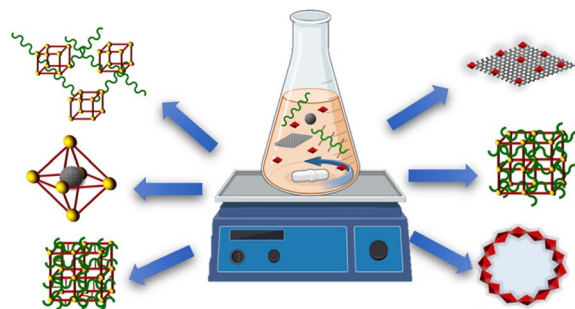
Zheliang Yuan* and Robert Britton*



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*



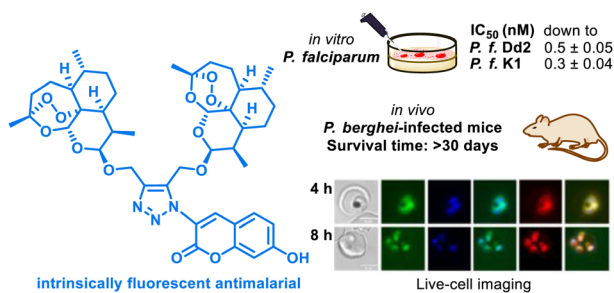
12926

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*



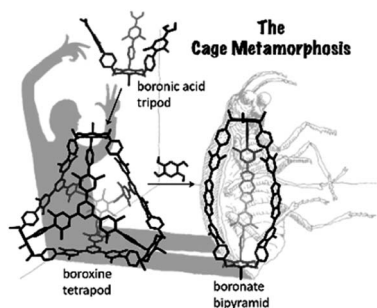
12941



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*

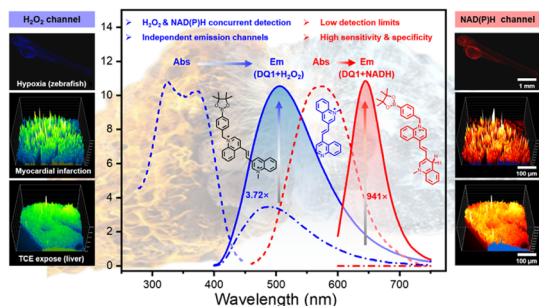
12953



Conformational control enables boroxine-to-boronate cage metamorphosis

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

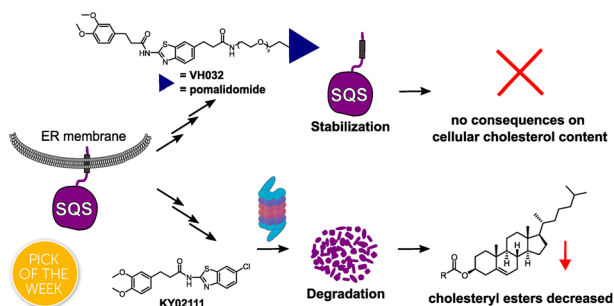
12961



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

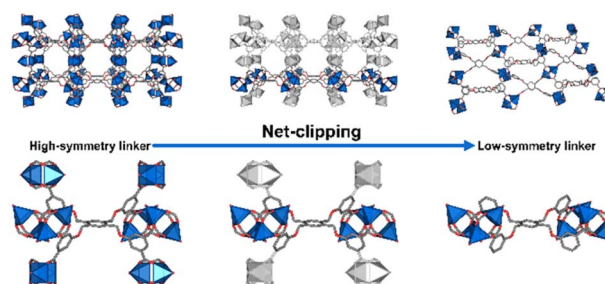
Joseph G. F. Hoock, Cecilia Rossetti, Mesut Bilgin, Laura Depta, Kasper Enemark-Rasmussen, John C. Christianson and Luca Laraia*



12984

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

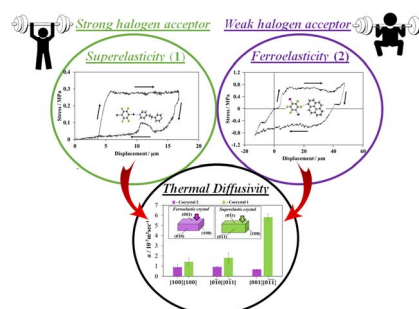
Borja Ortín-Rubio, Jaume Rostoll-Berenguer, Carlos Vila, Davide M. Proserpio, Vincent Guillerm, Judith Juanhuix, Inhar Imaz* and Daniel Maspoch*



12995

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

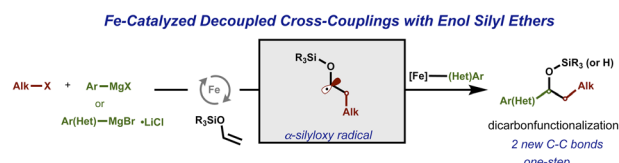
Subham Ranjan, Ryota Morioka, Meguya Ryu, Junko Morikawa* and Satoshi Takamizawa*



13007

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

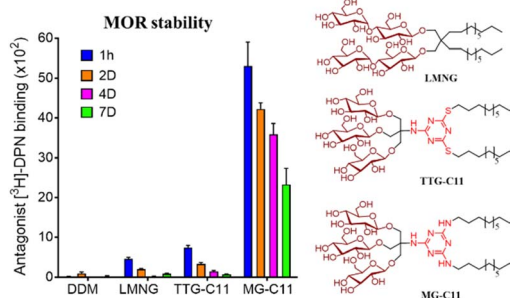
Dinabandhu Sar, Shuai Yin, Jacob Grygus, Ángel Rentería-Gómez, Melanie Garcia and Osvaldo Gutierrez*



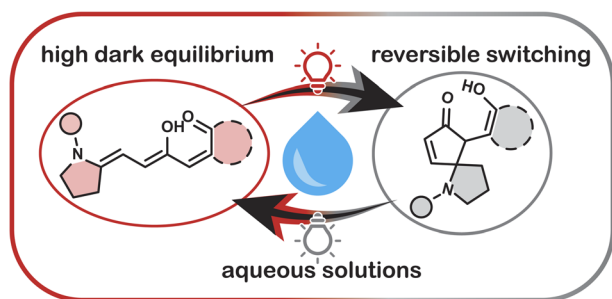
13014

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*



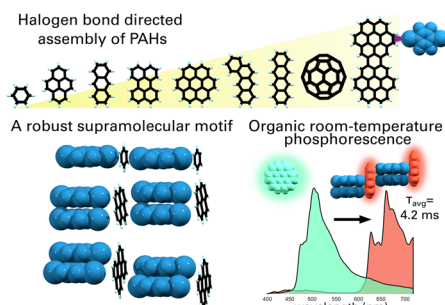
13025



Tethered together: DASA design towards aqueous compatibility

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

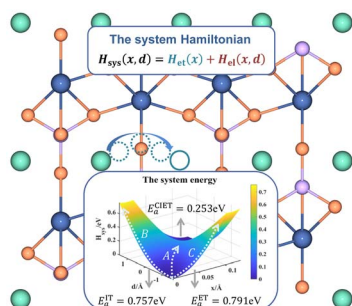
13031



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

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

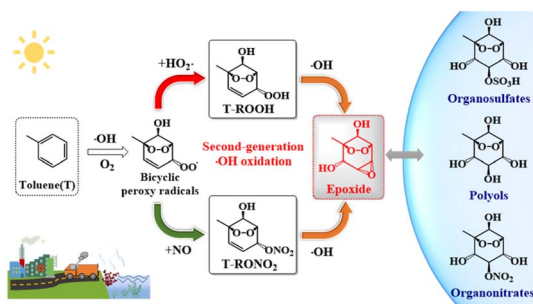
13042



The decisive role of electrostatic interactions in transport mode and phase segregation of lithium ions in LiFePO₄

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

13050

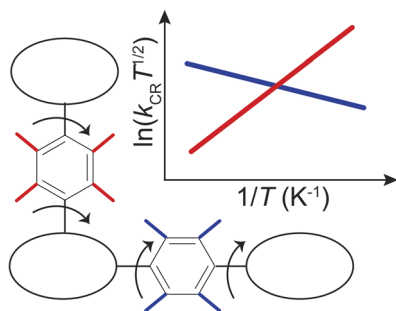


An overlooked oxidation mechanism of toluene: computational predictions and experimental validations

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*



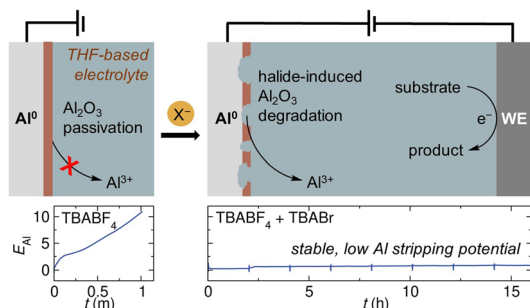
13095



Anti-Arrhenius behavior of electron transfer reactions in molecular dimers

Neo Lin and Tomoyasu Mani*

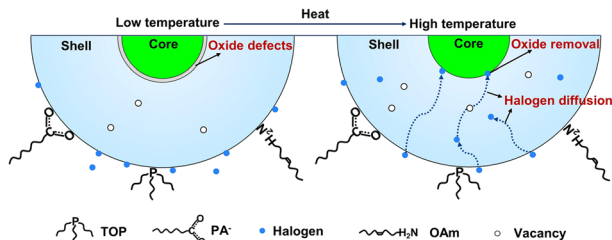
13108



Enabling Al sacrificial anodes in tetrahydrofuran electrolytes for reductive electrochemistry

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

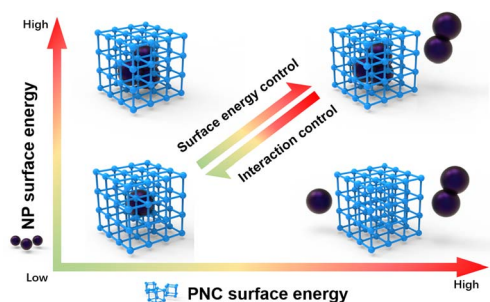
13119



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

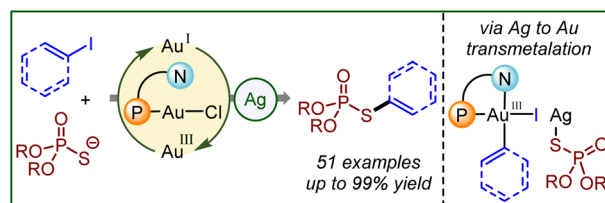
Li Zhou, Yuanyuan An, Jialong Ma, Guoxiu Hao, Zhehui Li, Junchen Chen and Lien-Yang Chou*



13134

Gold-catalyzed alkenylation and arylation of phosphorothioates

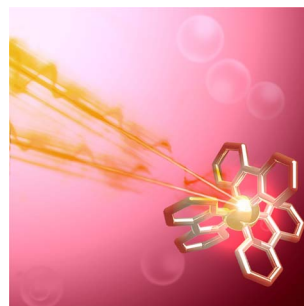
Urvashi, Sampurna Mishra and Nitin T. Patil*



13140

Observation of parallel intersystem crossing and charge transfer-state dynamics in [Fe(bpy)₃]²⁺ from ultrafast 2D electronic spectroscopy

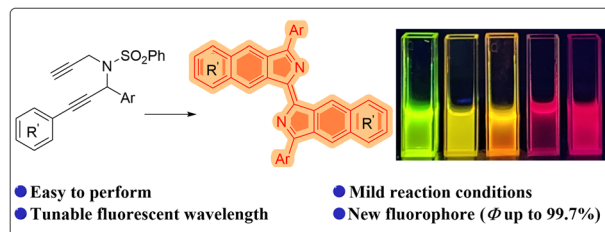
Angela Lee, Minjung Son, Mawuli Deegbey, Matthew D. Woodhouse, Stephanie M. Hart, Hayden F. Beissel, Paul T. Cesana, Elena Jakubikova, James K. McCusker* and Gabriela S. Schlau-Cohen*



13151

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

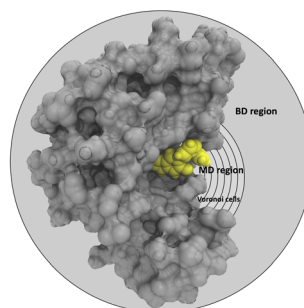
Changqing Ye, Rui Huang, Mong-Feng Chiou, Bo Wang, Daliang Li* and Hongli Bao*



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*



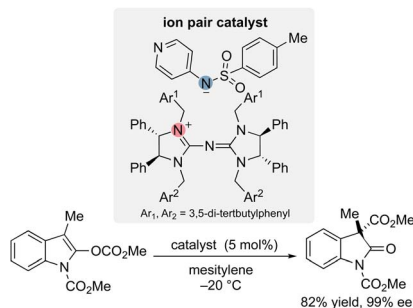
13176



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*

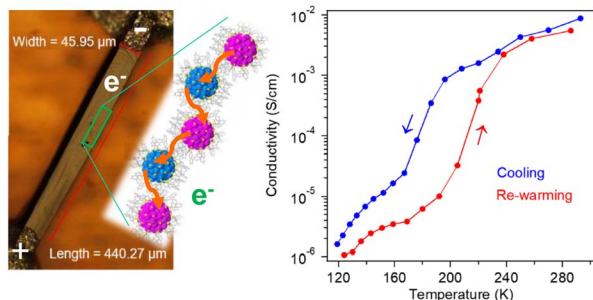
13184



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 bistability 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

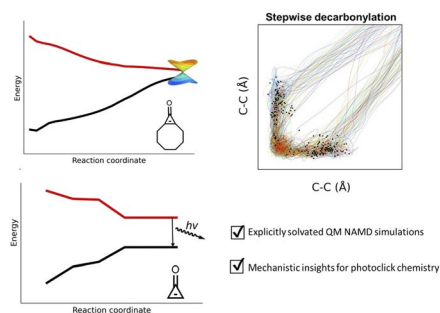
Shunhan Jia, Xingxing Tan, Limin Wu, Xiaodong Ma, Libing Zhang, Jiaqi Feng, Liang Xu, Xinning Song, Qinggong Zhu, Xinchen Kang, Xiaofu Sun* and Buxing Han*



13205

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

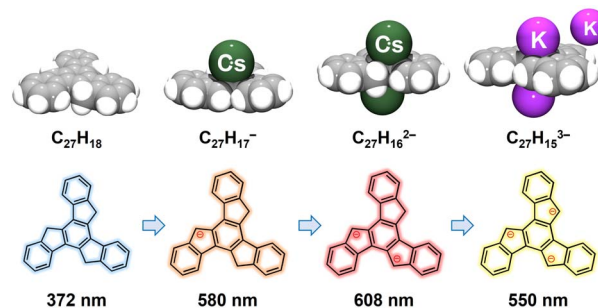
Daniel M. Adrion, Waruni V. Karunaratne and Steven A. Lopez*



13219

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

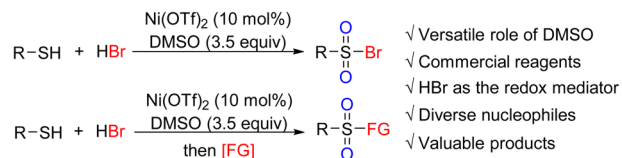
Yumeng Guo, Herdya S. Torchon, Yikun Zhu, Zheng Wei, Zhenyi Zhang, Haixiang Han,* Marina A. Petrukhina* and Zheng Zhou*



13228

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

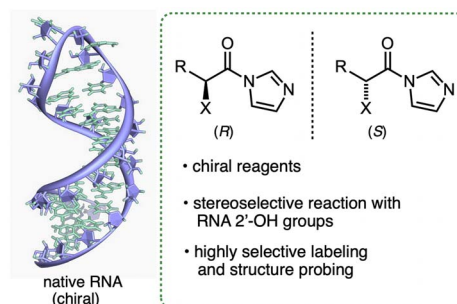
Hongye Wang, Zhaoting Li, Rongheng Dai, Ning Jiao and Song Song*



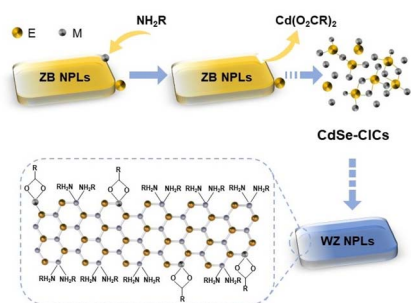
13235

Stereoselective RNA reaction with chiral 2'-OH acylating agents

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



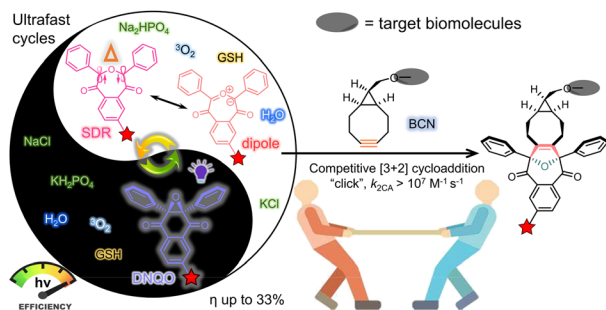
13244



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*

