

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 16(1) 1–452 (2025)



Cover
See Chonghuan Zhang, Kuangbiao Liao *et al.*, pp. 43–56. Image reproduced by permission of Chonghuan Zhang and Kuangbiao Liao from *Chem. Sci.*, 2025, 16, 43.



Inside cover
See Trinidad Novoa, Julia Contreras-García *et al.*, pp. 57–68. Image reproduced by permission of Francisca J. Benitez from *Chem. Sci.*, 2025, 16, 57.

EDITORIAL

17

Celebrating 15 years of *Chemical Science*!

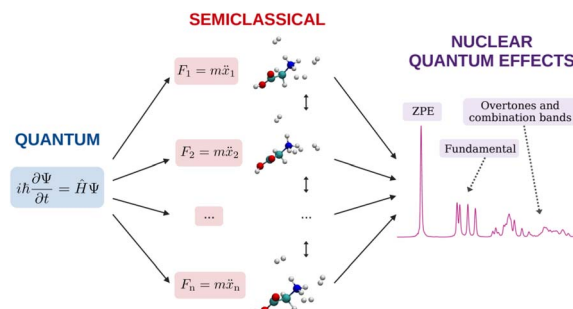


PERSPECTIVE

20

Semiclassical description of nuclear quantum effects in solvated and condensed phase molecular systems

Riccardo Conte,^{*} Giacomo Mandelli, Giacomo Botti, Davide Moscato, Cecilia Lanzi, Marco Cazzaniga,^{*} Chiara Aieta^{*} and Michele Ceotto^{*}



**GOLD
OPEN
ACCESS**

EES Batteries

**Exceptional research on
batteries and energy storage**

Part of the EES family

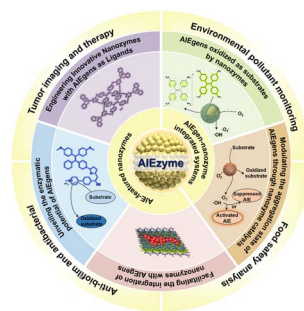
**Join
in** | Publish with us
rsc.li/EESBatteries

REVIEW

29

Recent advances in emerging nanozymes with aggregation-induced emission

Xin Li, Zhao Wang, Jing He, Haitham Al-Mashriqi, Jia Chen* and Hongdeng Qiu*



EDGE ARTICLES

43

SynAsk: unleashing the power of large language models in organic synthesis

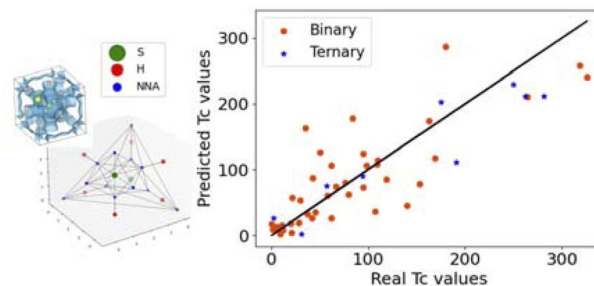
Chonghuan Zhang, Qianghua Lin, Biwei Zhu, Haopeng Yang, Xiao Lian, Hao Deng, Jiajun Zheng and Kuangbiao Liao*



57

TcESTIME: predicting high-temperature hydrogen-based superconductors

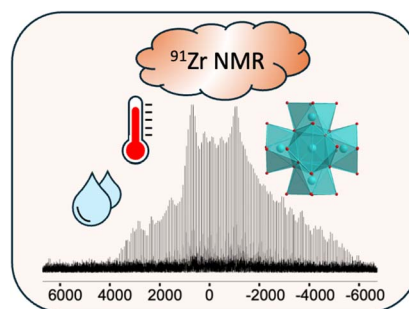
Trinidad Novoa,* Matias E. di Mauro, Diego Inostroza, Kaoutar El Haloui, Nicolas Sisourat, Yvon Maday and Julia Contreras-García*



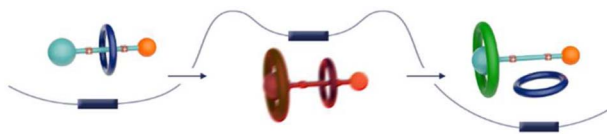
69

Probing the water adsorption and stability under steam flow of Zr-based metal-organic frameworks using ^{91}Zr solid-state NMR spectroscopy

Athulya Nadol, Florian Venel, Raynald Giovine, Maëva Leloire, Christophe Volkringer, Thierry Loiseau, Christel Gervais, Caroline Mellot-Draznieks, Bertrand Doumert, Julien Trébosc, Olivier Lafon and Frédérique Pourpoint*



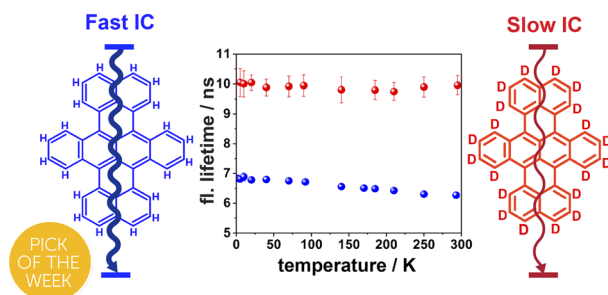
83



Allosteric release of cucurbit[6]uril from a rotaxane using a molecular signal

Aneta Závodná, Petr Janovský, Václav Kolařík, Jas S. Ward, Zdeňka Prucková, Michal Rouchal, Kari Rissanen and Robert Vícha*

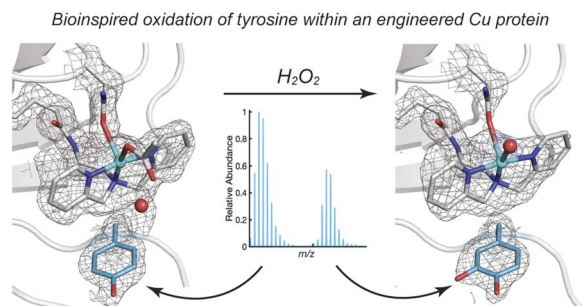
90



Suppressing non-radiative relaxation in a NIR single photon emitter: the impact of deuteration and temperature

Krishna Mishra, Zehua Wu, Christian Erker, Klaus Müllen and Thomas Basché*

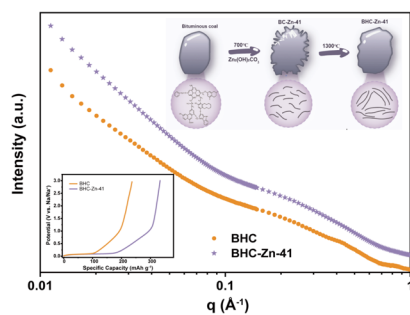
98



Selective oxidation of active site aromatic residues in engineered Cu proteins

Kylie S. Uyeda, Alec H. Follmer* and A. S. Borovik*

104



Breakage of the dense structure of coal precursors increases the plateau capacity of hard carbon for sodium storage

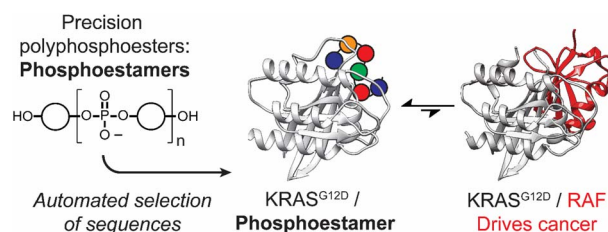
Wen-Yu Qian, Xin-Yang Zhou, Xin-Yao Liu, Meng-Yuan Su, Kai-Yang Zhang and Xing-Long Wu*



113

Sequence-defined phosphoestamers for selective inhibition of the KRAS^{G12D}/RAF1 interaction

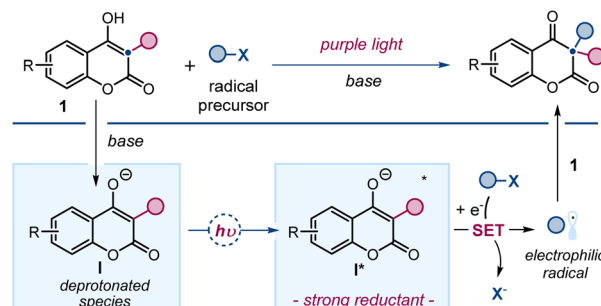
Bini Claringbold, Steven Vance, Alexandra R. Paul, James Williamson, Michelle D. Garrett* and Christopher J. Serpell*



124

Radical pathways for 2,4-chromandione synthesis via photoexcitation of 4-hydroxycoumarins

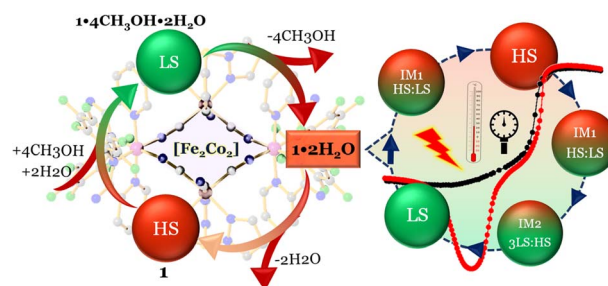
Sumitava Mallik, Enrico Sfreddo, Hailong Wang and Paolo Melchiorre*



130

Spin state modulation and kinetic control of thermal contraction in a [Fe₂Co₂] discrete Prussian blue analogue

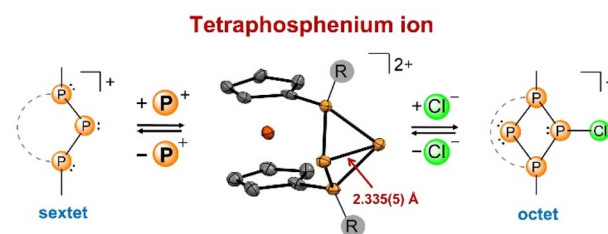
Jyoti Yadav and Sanjit Konar*



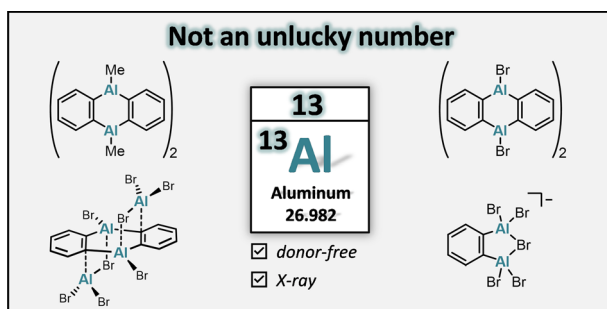
139

P⁺ addition and transfer involving a tetraphosphenium ion

Roman Franz, Máté Bartek, Clemens Bruhn, Zsolt Kelemen* and Rudolf Pietschnig*



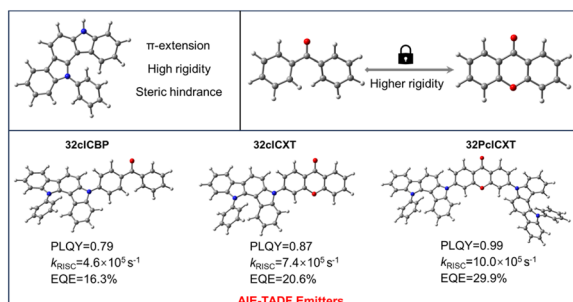
147



Donor-free 9,10-dihydro-9,10-dialuminaanthracenes

Paula L. Lückert, Jannik Gilmer, Alexander Virovets, Hans-Wolfram Lerner and Matthias Wagner*

156

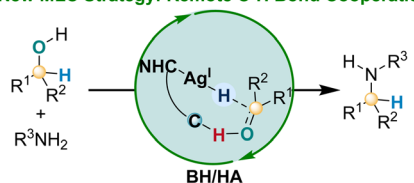


An effective design strategy for thermally activated delayed fluorescence emitters with aggregation-induced emission to enable sky-blue OLEDs that achieve an EQE of nearly 30%

Hui Dai, Yaohui Liang, Xiang Long, Tianyi Tang, Haozhi Xie, Zhiwei Ma, Gaoyu Li, Zhan Yang,* Juan Zhao* and Zhenguo Chi*

163

New MLC Strategy: Remote C-H Bond Cooperation

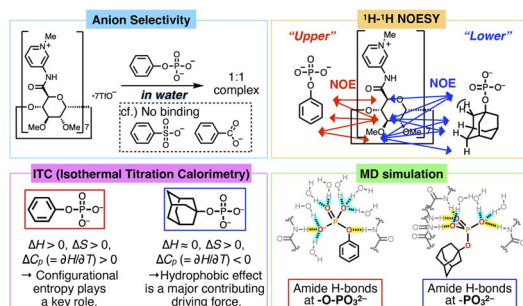


- first Ag(I)-catalyzed BH/HA N-alkylation reaction
- enable remote cooperation in linear coordination
- avoid poisoning by covalent C-H bond assistance
- tuning silver-hydride reactivity on *trans*-position

Remote C-H bond cooperation strategy enabled silver catalyzed borrowing hydrogen reactions

Zhe Chen, Laofeng Ouyang, Ning Wang, Weikang Li and Zhuofeng Ke*

171



Amide cyclodextrin that recognises monophosphate anions in harmony with water molecules

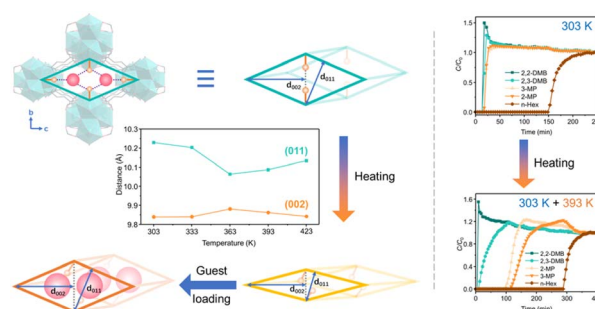
Takashi Nakamura,* Hayato Takayanagi, Masaki Nakahata,* Takumi Okubayashi, Hitomi Baba, Yoshiki Ishii, Go Watanabe,* Daisuke Tanabe and Tatsuya Nabeshima



182

Synergistic global and local flexibilities in Zr-based metal–organic frameworks enable sequential sieving of hexane isomers

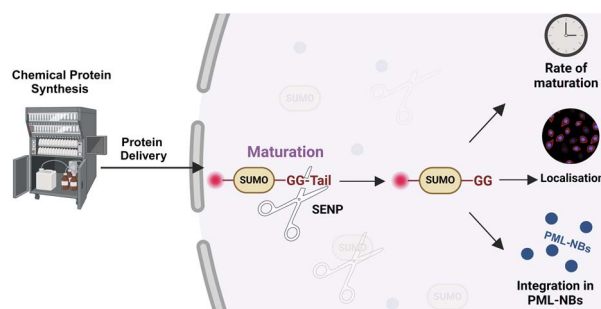
Rundao Chen, Jiaqi Li, Fang Zheng,* Fangru Zhou, Bin Sheng, Baojian Liu, Qiwei Yang, Zhiguo Zhang, Qilong Ren and Zongbi Bao*



191

Chemical protein synthesis combined with protein cell delivery reveals new insights on the maturation process of SUMO2

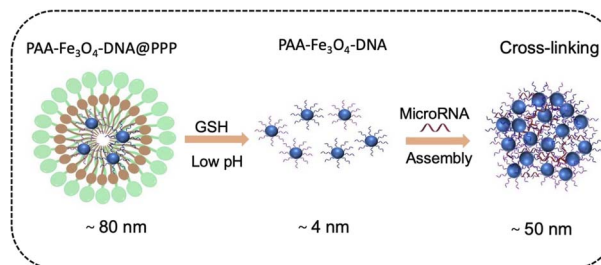
Dana Shkolnik, Subhasis Dey, Mahdi Hasan, Michael J. Matunis and Ashraf Brik*



199

A switchable magnetic resonance imaging nanoplatform for *in situ* microRNA imaging

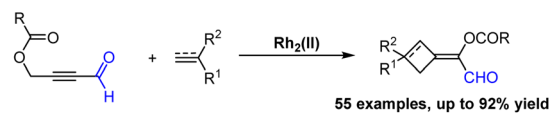
Yan Tan, Junren Wang, Qian Wan, Jinlong Yang, Jinkun Huang, Zijia Zhou, Haifeng Dong* and Xueji Zhang*



205

Tandem Rh(II)-catalyzed 1,3-acyloxy migration/intermolecular [2 + 2] cycloaddition of electron-deficient propargylic esters with alkenes and alkynes

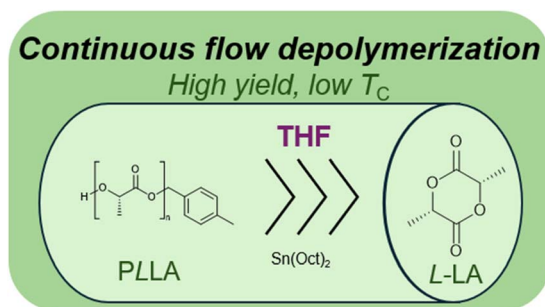
Zurong Xu, Dong Zhu, Rui Wu* and Shifa Zhu*



- Rh(II)-catalyzed 1,3-acyl migration of electronically deficient propargylic esters
- Tandem 1,3-acyl migration/intermolecular [2+2] cycloaddition
- Highly functionalized alkydenecyclobutane/ene products
- Operationally simple, broad substrate scope



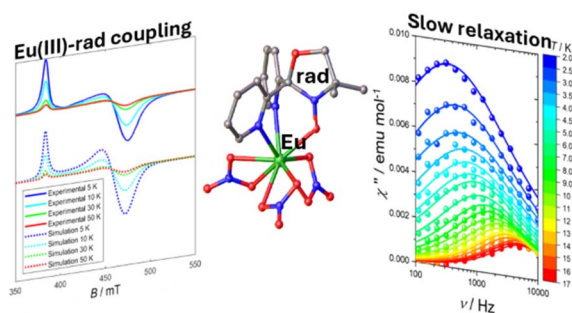
211



Depolymerisation of poly(lactide) under continuous flow conditions

Sophie Ellis, Antoine Buchard* and Tanja Junkers*

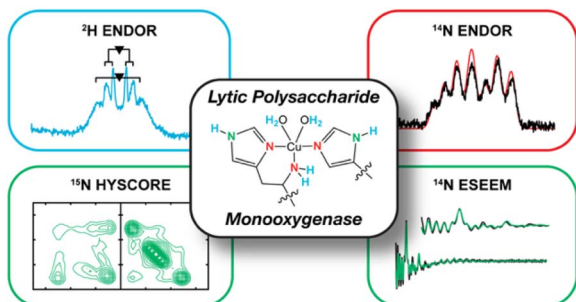
218



Slow magnetic relaxation and strong magnetic coupling in the nitroxyl radical complexes of lanthanide(III) with diamagnetic ground state ($\text{Ln} = \text{Lu}, \text{Eu}$)

Lorenzo Sorace, Alexey A. Dmitriev, Mauro Perfetti* and Kira E. Vostrikova*

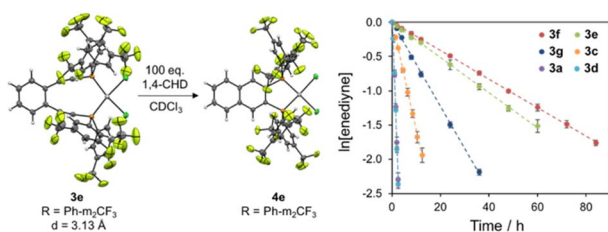
233



pH-mediated manipulation of the histidine brace in LPMOs and generation of a tri-anionic variant, investigated by EPR, ENDOR, ESEEM and HSCORE spectroscopy

Julia Haak, Ole Goltjen, Morten Sørli, Vincent G. H. Eijsink and George E. Cutsail III*

255



Pronounced electronic modulation of geometrically-regulated metallacyclopentadiene cyclization

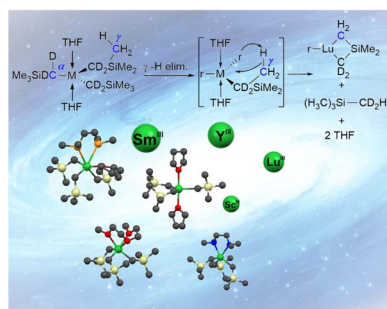
Sarah E. Lindahl, Erin M. Metzger, Chun-Hsing Chen, Maren Pink and Jeffrey M. Zaleski*



280

Stabilization of reactive rare earth alkyl complexes through mechanistic studies

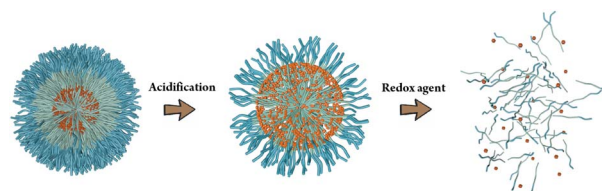
Elias Tanuhadi, Anna S. Bair, Mary Johnson, Philip Fontaine, Jerzy Klosin,* Sudipta Pal and Polly L. Arnold*



288

Facile construction of polyoxometalate-polymer hybrid nanoparticles with pH/redox dual-responsiveness

Yanting Gao, Fan Yang, Yufu Wang, Angus P. R. Johnston, Rebekah N. Duffin, Philip C. Andrews, Chris Ritchie* and Georgina K. Such*



297

An ultra-fast reaction process for recycling lithium ion batteries via galvanic cell interaction

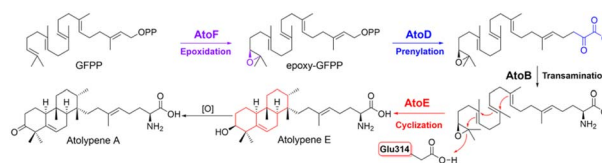
Long Ye, Zhilong Xu, Haiqiang Gong, Zhiming Xiao, Bao Zhang, Lei Ming and Xing Ou*



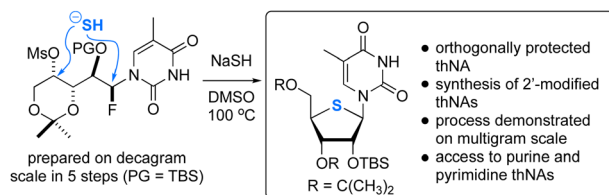
310

Biosynthesis of a bacterial meroterpenoid reveals a non-canonical class II meroterpenoid cyclase

Zengyuan Wang, Tyler A. Alsup, Xingming Pan, Lu-Lu Li, Jupeng Tian, Ziyi Yang, Xiaoxu Lin, Hui-Min Xu, Jeffrey D. Rudolf and Liao-Bin Dong*



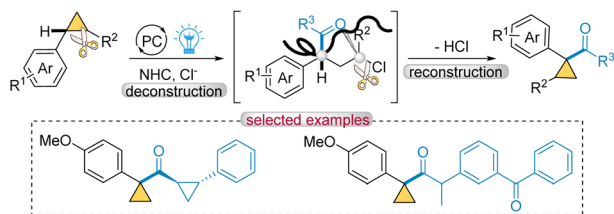
318



A flexible and scalable synthesis of 4'-thionucleosides

Callum Lucas, Ethan Fung, Matthew Nodwell, Steven Silverman, Bara Singh, Louis-Charles Campeau and Robert Britton*

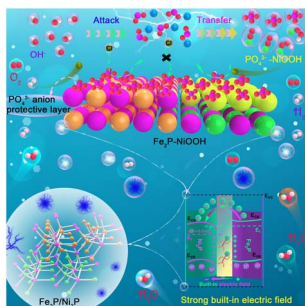
323



Cooperative photoredox and N-heterocyclic carbene-catalyzed formal C–H acylation of cyclopropanes *via* a deconstruction–reconstruction strategy

Fan Gao, Tian Wang and Xiaoyu Yan*

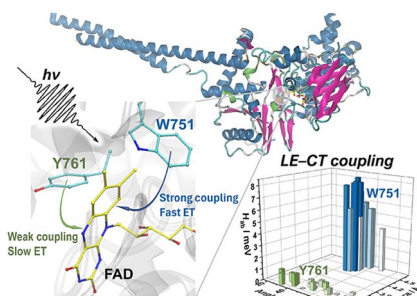
329



Modulating built-in electric field *via* Br induced partial phase transition for robust alkaline freshwater and seawater electrolysis

Lei Jin, Hui Xu,* Kun Wang, Yang Liu, Xingyue Qian, Haiqun Chen* and Guangyu He*

338



Mechanism of ultrafast flavin photoreduction in the active site of flavoenzyme LSD1 histone demethylase

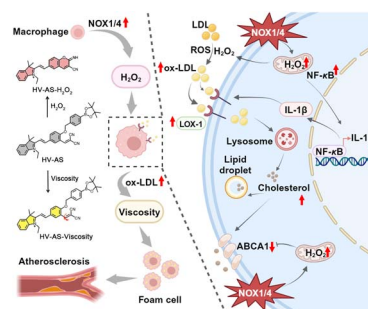
Bo Zhuang,* Rivo Ramodiharilafy, Alexey Aleksandrov,* Ursula Liebl and Marten H. Vos*



345

H₂O₂ accumulation promoting internalization of ox-LDL in early atherosclerosis revealed via a synergistic dual-functional NIR fluorescence probe

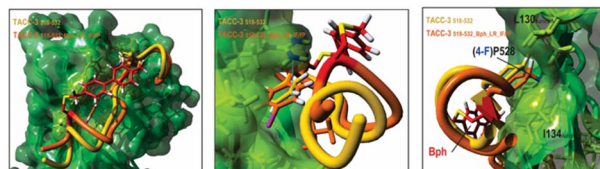
Hui Wang,* Jingjing Guo, Tiancong Xiu, Yue Tang,*
Ping Li,* Wei Zhang, Wen Zhang and Bo Tang*



354

Constrained TACC3 peptidomimetics for a non-canonical protein–protein interface elucidate allosteric communication in Aurora-A kinase

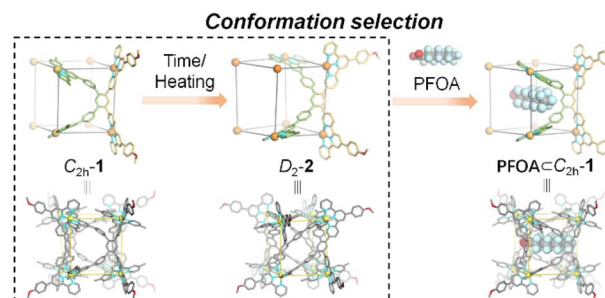
Diana Gimenez, Martin Walko, Jennifer A. Miles,
Richard Bayliss,* Megan H. Wright* and Andrew J. Wilson*



364

Dynamic selection in metallo-organic cube Cd₈L₄ conformations induced by perfluorooctanoate encapsulation

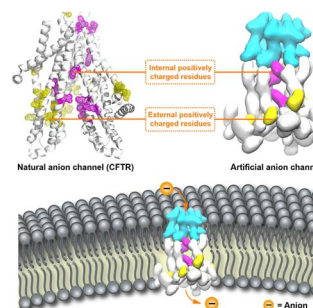
Yu-Qing Li, He Zhao, Ermeng Han, Zhiyuan Jiang,*
Qixia Bai, Yu-Ming Guan, Zhe Zhang, Tun Wu*
and Pingshan Wang*



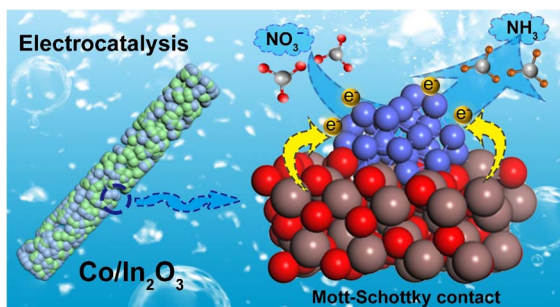
371

Synthetic anion channels: achieving precise mimicry of the ion permeation pathway of CFTR in an artificial system

Linlin Mao, Shuaimin Hou, Linlin Shi, Jingjing Guo,*
Bo Zhu, Yonghui Sun,* Junbiao Chang and Pengyang Xin*



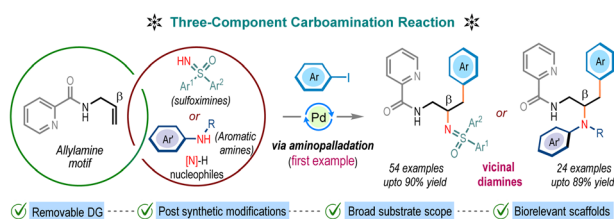
378



Enhanced electrocatalytic nitrate-to-ammonia performance from Mott–Schottky design to induce electron redistribution

Ruikai Qi, Qiuling Jiang, Li Deng, Xianqiang Yu, Bingyan Shi, Mengxiao Zhong,* Ying Wang* and Xiaofeng Lu*

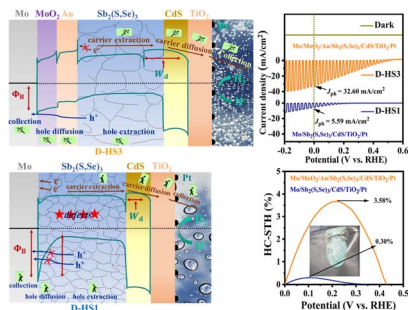
386



Regioselective intermolecular carboamination of allyl amines via nucleopalladation: empowering three-component synthesis of vicinal diamines

Shib Nath Saha, Nityananda Ballav, Suman Ghosh and Mahiuddin Baidya*

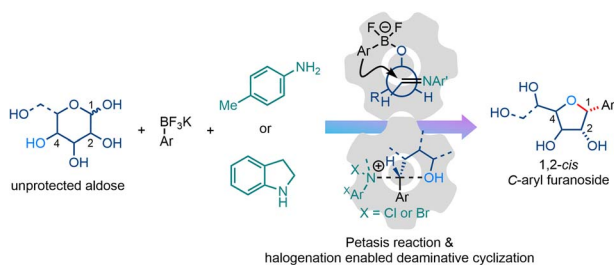
393



Dual back interface engineering optimized charge carrier dynamics in Sb₂(S,Se)₃ photocathodes for efficient solar hydrogen production

Hafiz Sartaj Aziz, Tahir Imran, Munir Ahmad, Guo-Jie Chen, Ping Luo, Dong-Lou Ren, Bing-Suo Zou, Ju-Guang Hu, Zheng-Hua Su, Pei-Guang Yan, Guang-Xing Liang and Shuo Chen*

410



Halogenation-induced C–N bond activation enables the synthesis of 1,2-*cis* C-aryl furanosides via deaminative cyclization

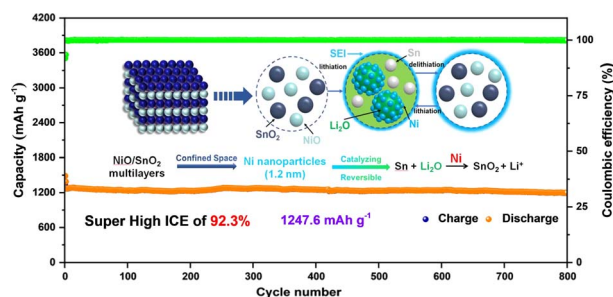
Wenbo Wang, Jiawei Wu, Kaiyu Jiang, Maochao Zhou and Gang He*



418

Spatially confined transition metals boost high initial coulombic efficiency in alloy anodes

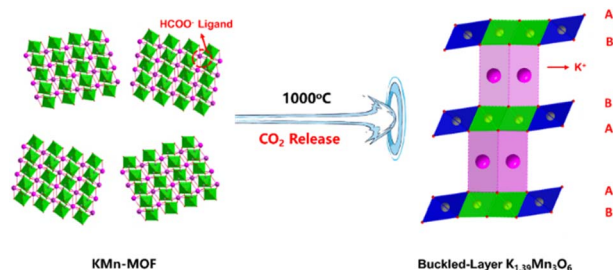
Haoyu Fu, Fangchao Gu, Yize Niu, Shuxuan Liao, Zeyuan Bu, Haonan Wang, Dong Yang, Xiaoshan Wang* and Qiang Li*



425

Buckled-layer K_{1.39}Mn₃O₆: a novel cathode for potassium-ion batteries

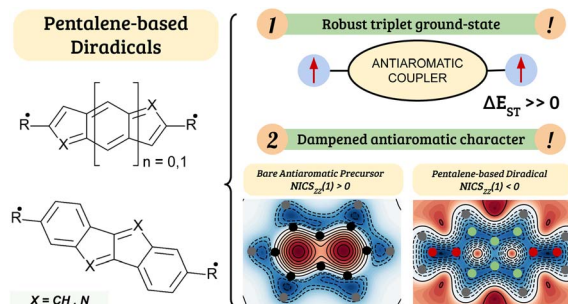
Ang Li, Ziqi Wang and Yunhua Xu*



430

Rational design of organic diradicals with robust high-spin ground state based on antiaromatic linkers

Raul Santiago,* M. Àngels Carvajal, Jordi Poater, Ibério de P. R. Moreira, Stefan T. Bromley, Mercè Deumal and Jordi Ribas-Ariño*



CORRECTIONS

448

Correction: Perylene-derivative singlet exciton fission in water solution

Chloe Magne, Simona Streckaite, Roberto A. Boto, Eduardo Domínguez-Ojeda, Marina Gromova, Andrea Echeverri, Flavio Siro Brigiano, Minh-Huong Ha-Thi, Marius Franckevičius, Vidmantas Jašinskas, Annamaria Quaranta, Andrew A. Pascal, Matthieu Koepf, David Casanova, Thomas Pino, Bruno Robert, Julia Contreras-García, Daniel Finkelstein-Shapiro, Vidmantas Gulbinas and Manuel J. Llansola-Portoles*



449

Correction: Ion pair extractant selective for LiCl and LiBr

Nam Jung Heo, Ju Hyun Oh, Aimin Li, Kyoungsoon Lee, Qing He, Jonathan L. Sessler* and Sung Kuk Kim*

