

# Chemical Science

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## IN THIS ISSUE

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**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

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**Celebrating 15 years of *Chemical Science*!**

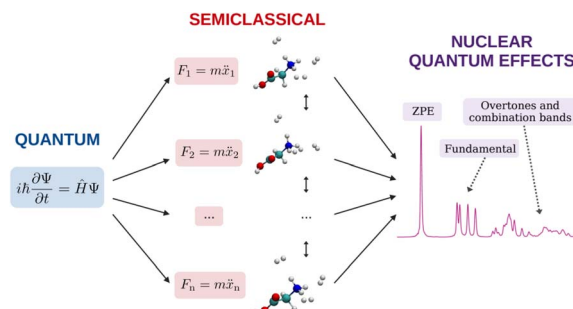


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Riccardo Conte,\* Giacomo Mandelli, Giacomo Botti, Davide Moscato, Cecilia Lanzi, Marco Cazzaniga,\* Chiara Aieta\* and Michele Ceotto\*



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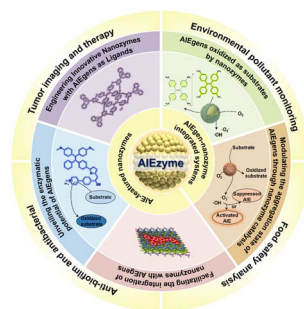
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Xin Li, Zhao Wang, Jing He, Haitham Al-Mashriqi, Jia Chen\* and Hongdeng Qiu\*



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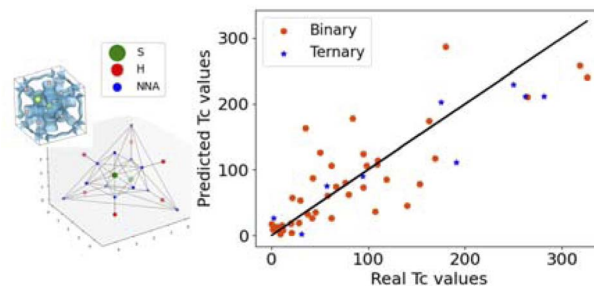
Chonghuan Zhang, Qianghua Lin, Biwei Zhu, Haopeng Yang, Xiao Lian, Hao Deng, Jiajun Zheng and Kuangbiao Liao\*



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**TcESTIME: predicting high-temperature hydrogen-based superconductors**

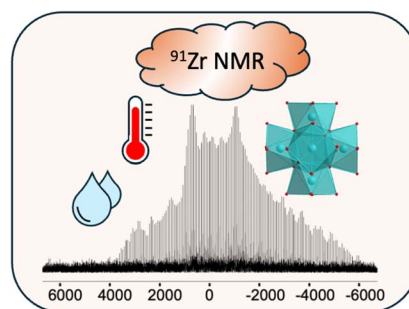
Trinidad Novoa,\* Matias E. di Mauro, Diego Inostroza, Kaoutar El Haloui, Nicolas Sisourat, Yvon Maday and Julia Contreras-García\*



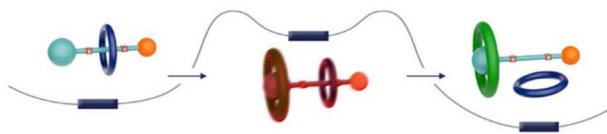
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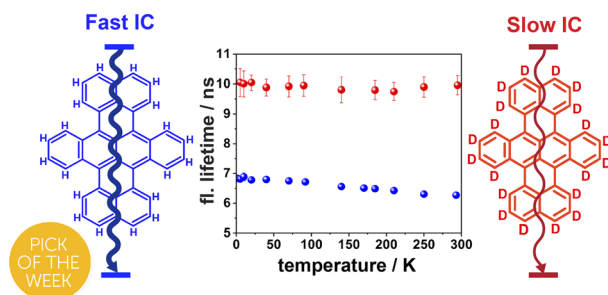
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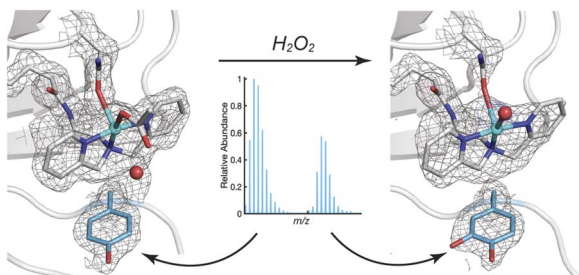


### Suppressing non-radiative relaxation in a NIR single photon emitter: the impact of deuteration and temperature

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

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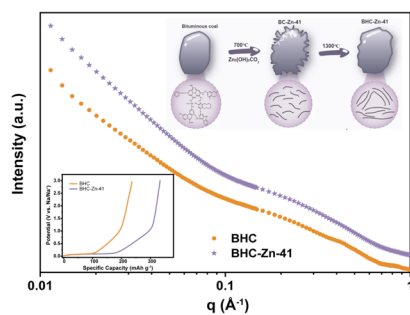
Bioinspired oxidation of tyrosine within an engineered Cu protein



### Selective oxidation of active site aromatic residues in engineered Cu proteins

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

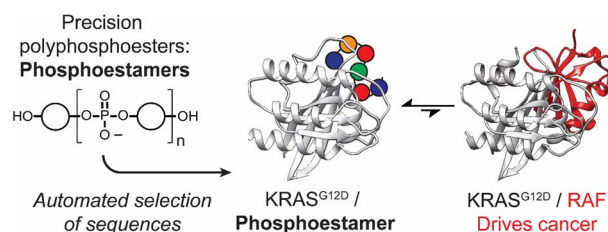
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### Sequence-defined phosphoestamers for selective inhibition of the KRAS<sup>G12D</sup>/RAF1 interaction

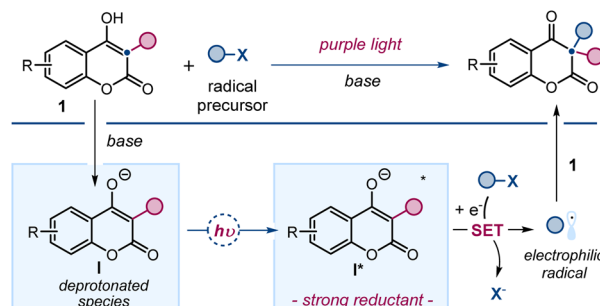
Bini Claringbold, Steven Vance, Alexandra R. Paul, James Williamson, Michelle D. Garrett\* and Christopher J. Serpell\*



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

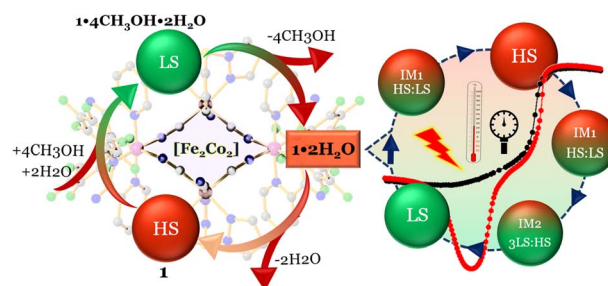
Sumitava Mallik, Enrico Sfreddo, Hailong Wang and Paolo Melchiorre\*



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### Spin state modulation and kinetic control of thermal contraction in a [Fe<sub>2</sub>Co<sub>2</sub>] discrete Prussian blue analogue

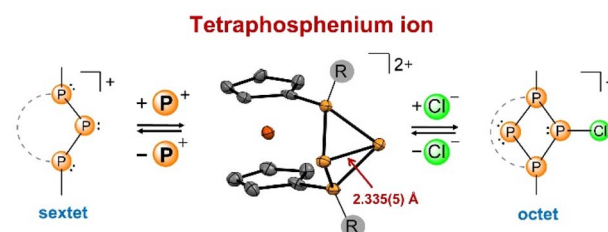
Jyoti Yadav and Sanjit Konar\*



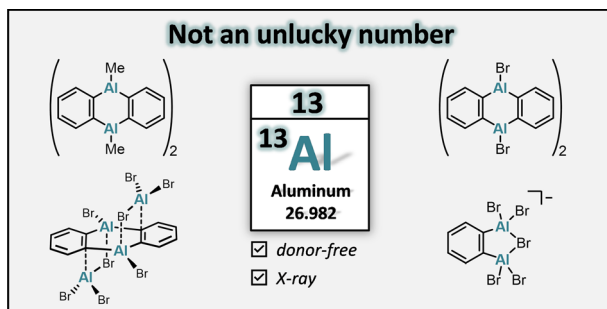
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### P<sup>+</sup> addition and transfer involving a tetraphosphenium ion

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



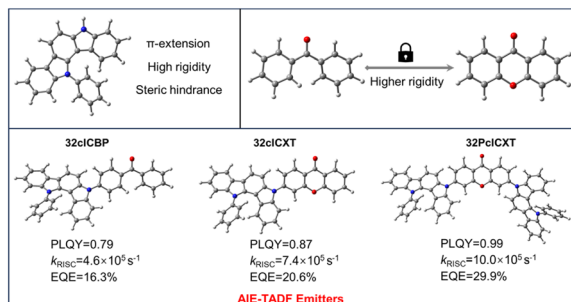
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### Donor-free 9,10-dihydro-9,10-dialuminaanthracenes

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

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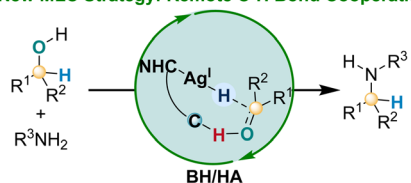


### An effective design strategy for thermally activated delayed fluorescence emitters with aggregation-induced emission to enable sky-blue OLEDs that achieve an EQE of nearly 30%

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

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#### New MLC Strategy: Remote C-H Bond Cooperation

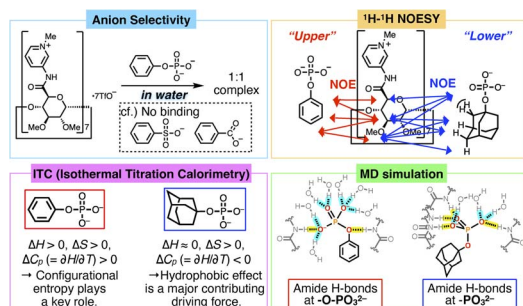


- first Ag(I)-catalyzed BH/HA *N*-alkylation reaction
- enable remote cooperation in linear coordination
- avoid poisoning by covalent C-H bond assistance
- tuning silver-hydride reactivity on *trans*-position

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

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

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### Amide cyclodextrin that recognises monophosphate anions in harmony with water molecules

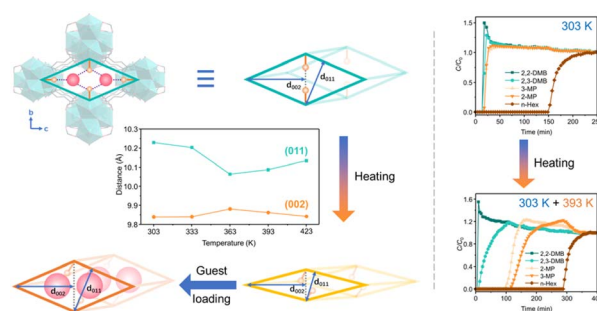
Takashi Nakamura,\* Hayato Takayanagi, Masaki Nakahata,\* Takumi Okubayashi, Hitomi Baba, Yoshiki Ishii, Go Watanabe,\* Daisuke Tanabe and Tatsuya Nabeshima



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

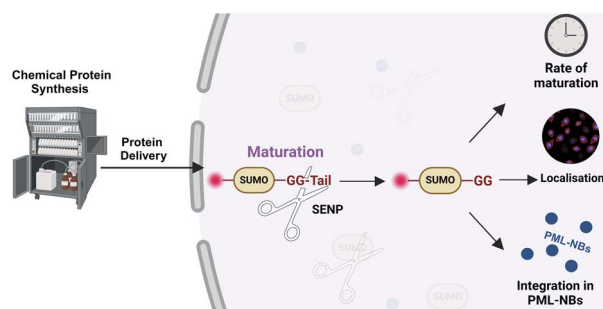
Rundao Chen, Jiaqi Li, Fang Zheng,\* Fangru Zhou, Bin Sheng, Baojian Liu, Qiwei Yang, Zhiguo Zhang, Qilong Ren and Zongbi Bao\*



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

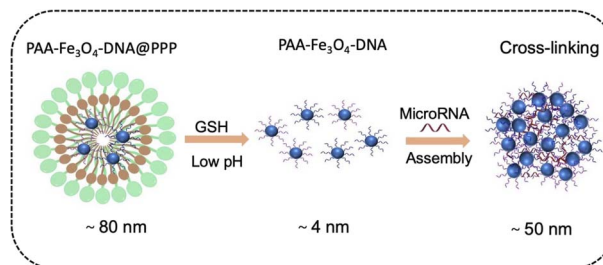
Dana Shkolnik, Subhasis Dey, Mahdi Hasan, Michael J. Matunis and Ashraf Brik\*



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

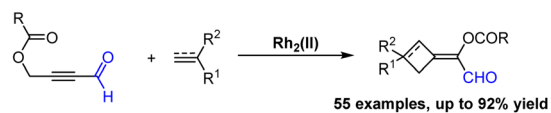
Yan Tan, Junren Wang, Qian Wan, Jinlong Yang, Jinkun Huang, Zijia Zhou, Haifeng Dong\* and Xueji Zhang\*



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

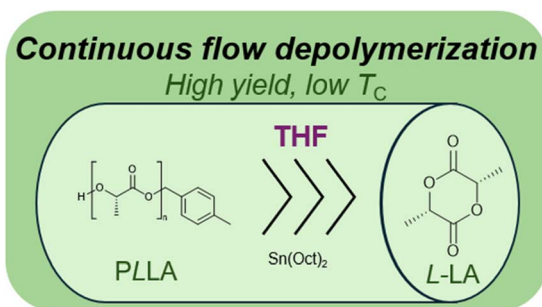
Zurong Xu, Dong Zhu, Rui Wu\* and Shifa Zhu\*



- 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



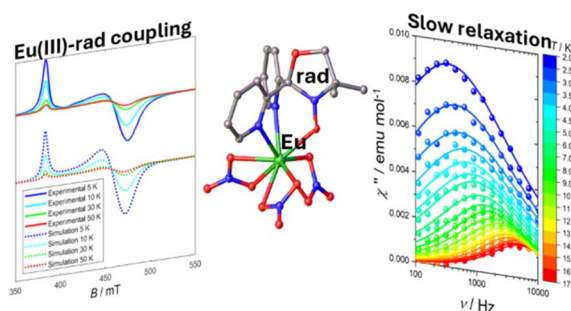
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### Depolymerisation of poly(lactide) under continuous flow conditions

Sophie Ellis, Antoine Buchard\* and Tanja Junkers\*

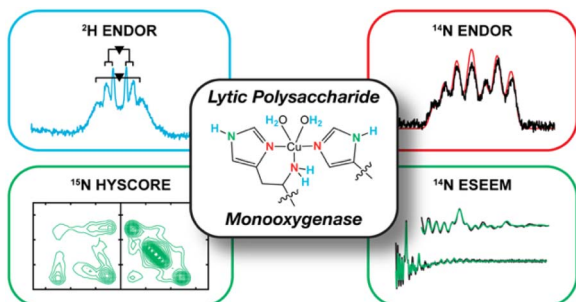
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### Slow magnetic relaxation and strong magnetic coupling in the nitroxyl radical complexes of lanthanide(III) with diamagnetic ground state (Ln = Lu, Eu)

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

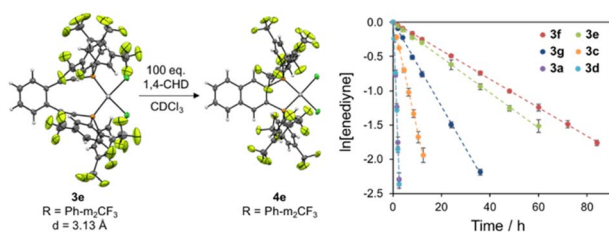
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### pH-mediated manipulation of the histidine brace in LPMOs and generation of a tri-anionic variant, investigated by EPR, ENDOR, ESEEM and HSCORE spectroscopy

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

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### Pronounced electronic modulation of geometrically-regulated metalloenediynes cyclization

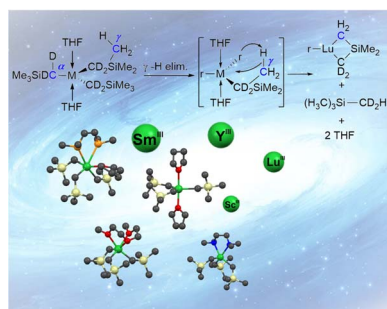
Sarah E. Lindahl, Erin M. Metzger, Chun-Hsing Chen, Maren Pink and Jeffrey M. Zaleski\*



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### Stabilization of reactive rare earth alkyl complexes through mechanistic studies

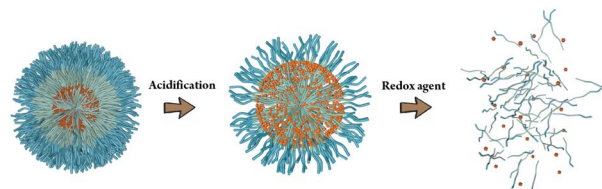
Elias Tanuhadi, Anna S. Bair, Mary Johnson, Philip Fontaine, Jerzy Klosin,\* Sudipta Pal and Polly L. Arnold\*



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

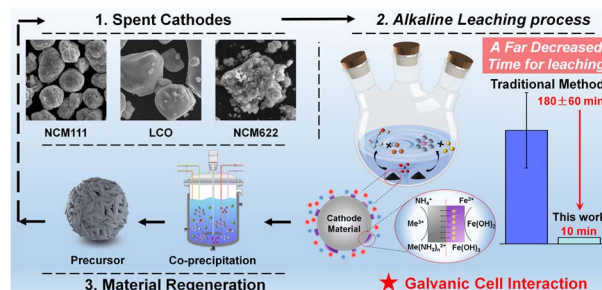
Yanting Gao, Fan Yang, Yufu Wang, Angus P. R. Johnston, Rebekah N. Duffin, Philip C. Andrews, Chris Ritchie\* and Georgina K. Such\*



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

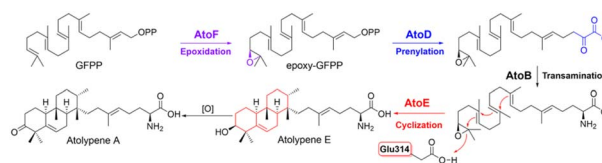
Long Ye, Zhilong Xu, Haiqiang Gong, Zhiming Xiao, Bao Zhang, Lei Ming and Xing Ou\*



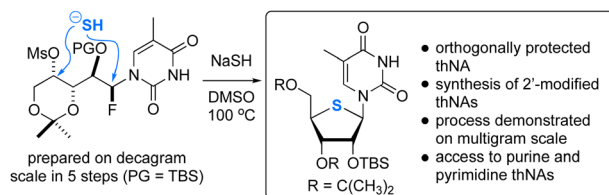
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### Biosynthesis of a bacterial meroterpenoid reveals a non-canonical class II meroterpenoid cyclase

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\*



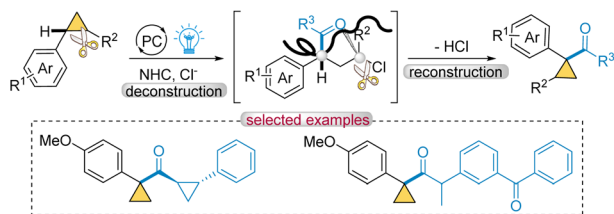
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### A flexible and scalable synthesis of 4'-thionucleosides

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

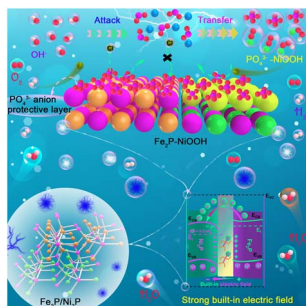
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### Cooperative photoredox and N-heterocyclic carbene-catalyzed formal C–H acylation of cyclopropanes *via* a deconstruction–reconstruction strategy

Fan Gao, Tian Wang and Xiaoyu Yan\*

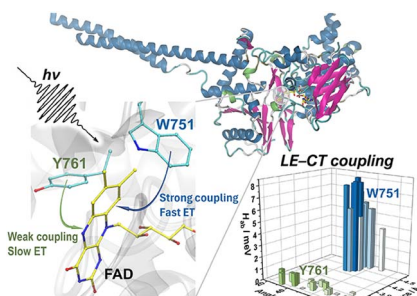
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### Modulating built-in electric field *via* Br induced partial phase transition for robust alkaline freshwater and seawater electrolysis

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

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

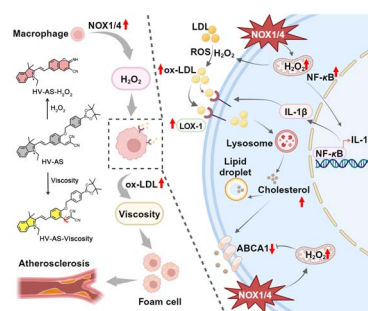
Bo Zhuang,\* Rivo Ramodiharilafy, Alexey Aleksandrov,\* Ursula Liebl and Marten H. Vos\*



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## H<sub>2</sub>O<sub>2</sub> accumulation promoting internalization of ox-LDL in early atherosclerosis revealed via a synergistic dual-functional NIR fluorescence probe

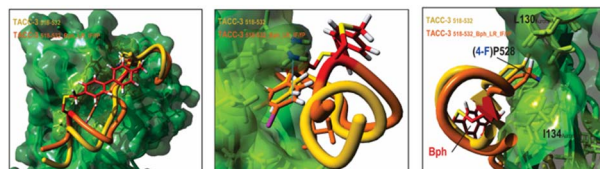
Hui Wang,\* Jingjing Guo, Tiancong Xiu, Yue Tang,\*  
Ping Li,\* Wei Zhang, Wen Zhang and Bo Tang\*



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

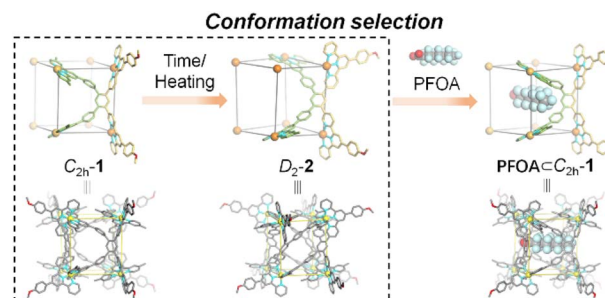
Diana Gimenez, Martin Walko, Jennifer A. Miles,  
Richard Bayliss,\* Megan H. Wright\* and Andrew J. Wilson\*



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## Dynamic selection in metallo-organic cube Cd<sub>8</sub>L<sub>4</sub> conformations induced by perfluorooctanoate encapsulation

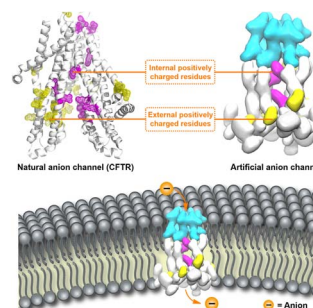
Yu-Qing Li, He Zhao, Ermeng Han, Zhiyuan Jiang,\*  
Qixia Bai, Yu-Ming Guan, Zhe Zhang, Tun Wu\*  
and Pingshan Wang\*



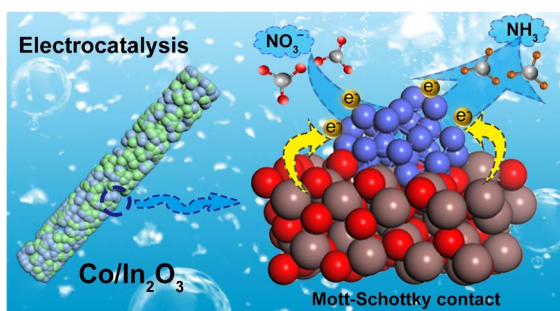
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## Synthetic anion channels: achieving precise mimicry of the ion permeation pathway of CFTR in an artificial system

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



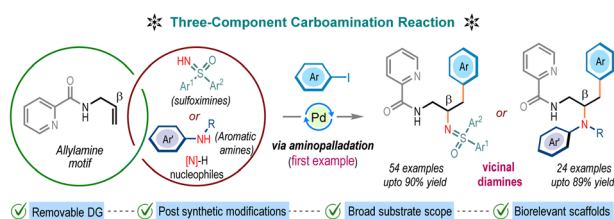
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### Enhanced electrocatalytic nitrate-to-ammonia performance from Mott–Schottky design to induce electron redistribution

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

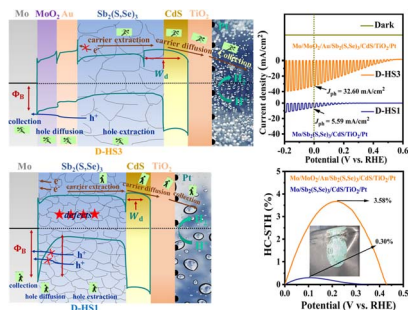
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### Regioselective intermolecular carboamination of allyl amines via nucleopalladation: empowering three-component synthesis of vicinal diamines

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

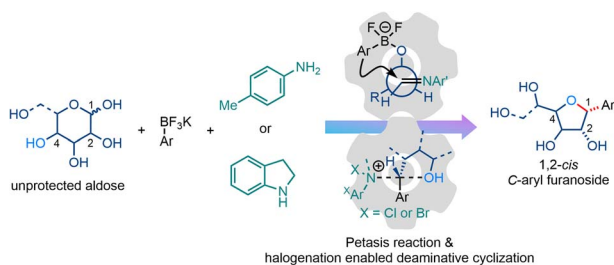
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### Dual back interface engineering optimized charge carrier dynamics in Sb<sub>2</sub>(S,Se)<sub>3</sub> photocathodes for efficient solar hydrogen production

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\*

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

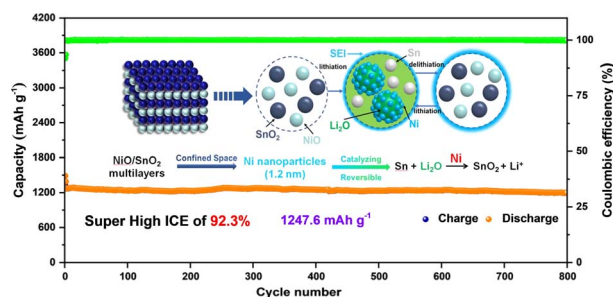
Wenbo Wang, Jiawei Wu, Kaiyu Jiang, Maochao Zhou and Gang He\*



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

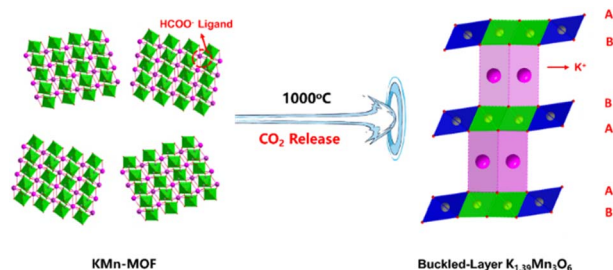
Haoyu Fu, Fangchao Gu, Yize Niu, Shuxuan Liao, Zeyuan Bu, Haonan Wang, Dong Yang, Xiaoshan Wang\* and Qiang Li\*



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### Buckled-layer K<sub>1.39</sub>Mn<sub>3</sub>O<sub>6</sub>: a novel cathode for potassium-ion batteries

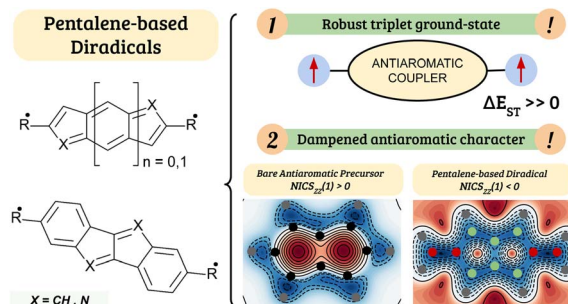
Ang Li, Ziqi Wang and Yunhua Xu\*



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### 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

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### 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\*



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**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\*

