

# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(1) 1–452 (2025)



### Cover

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Kuangbiao Liao *et al.*,  
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### Inside cover

See Trinidad Novoa, Julia  
Contreras-García *et al.*,  
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2025, **16**, 57.

## EDITORIAL

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

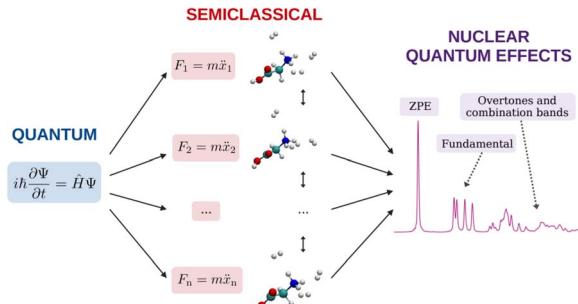


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### Semiclassical description of nuclear quantum effects in solvated and condensed phase molecular systems

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



# EES Batteries

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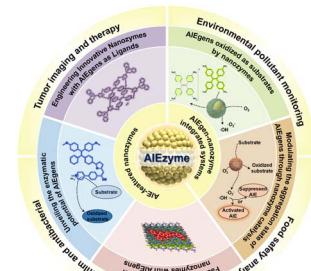
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## REVIEW

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## Recent advances in emerging nanozymes with aggregation-induced emission

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



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

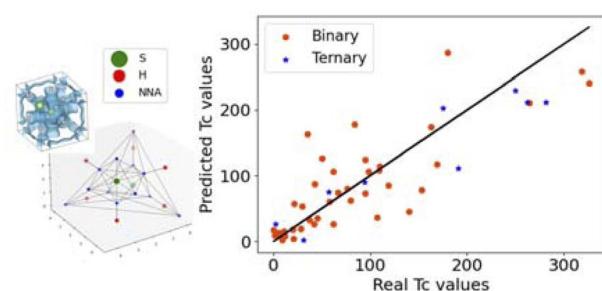
Chonghuan Zhang, Qianghua Lin, Biwei Zhu,  
Haopeng Yang, Xiao Lian, Hao Deng, Jiajun Zheng  
and Kuangbiao Liao\*



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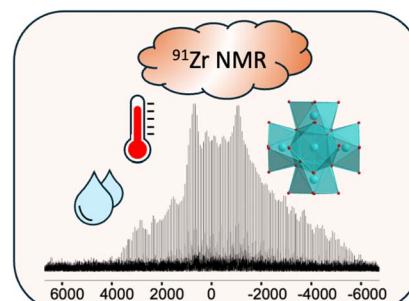
Trinidad Novoa,\* Matías E. di Mauro, Diego Inostroza,  
Kaoutar El Haloui, Nicolas Sisourat, Yvon Maday  
and Julia Contreras-García\*



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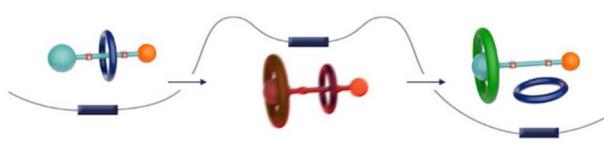
## Probing the water adsorption and stability under steam flow of Zr-based metal–organic frameworks using $^{91}\text{Zr}$ solid-state NMR spectroscopy

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



## EDGE ARTICLES

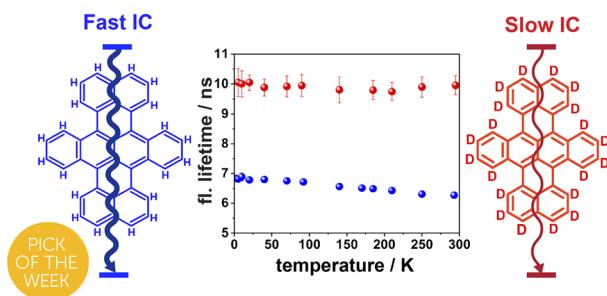
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### Allosteric release of cucurbit[6]uril from a rotaxane using a molecular signal

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

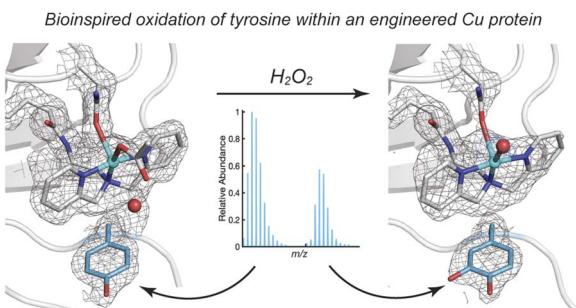
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### Suppressing non-radiative relaxation in a NIR single photon emitter: the impact of deuteration and temperature

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

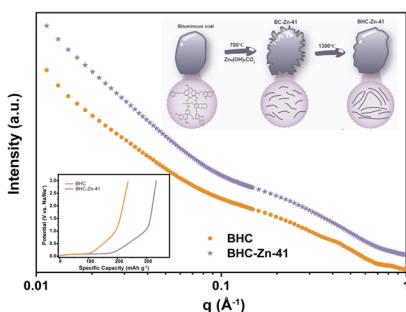
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Wen-Yu Qian, Xin-Yang Zhou, Xin-Yao Liu, Meng-Yuan Su, Kai-Yang Zhang and Xing-Long Wu\*

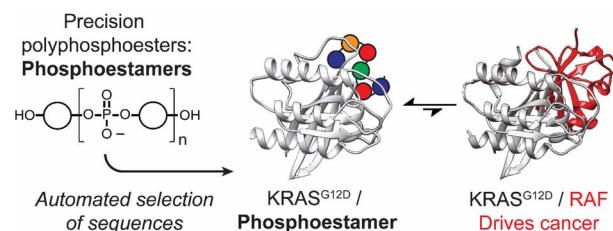


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**Sequence-defined phosphoestamers for selective inhibition of the KRAS<sup>G12D</sup>/RAF1 interaction**

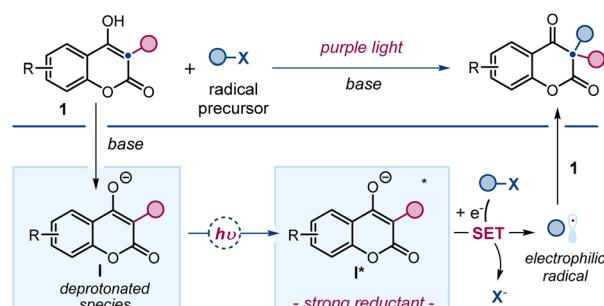
Bini Claringbold, Steven Vance, Alexandra R. Paul,  
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**Radical pathways for 2,4-chromandione synthesis via photoexcitation of 4-hydroxycoumarins**

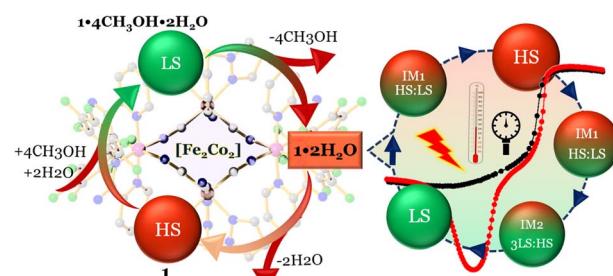
Sumitava Mallik, Enrico Sfreddo, Hailong Wang  
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**Spin state modulation and kinetic control of thermal contraction in a [Fe<sub>2</sub>Co<sub>2</sub>] discrete Prussian blue analogue**

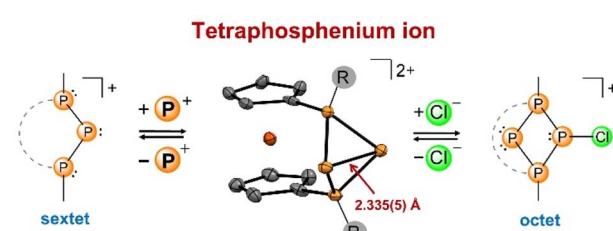
Jyoti Yadav and Sanjit Konar\*



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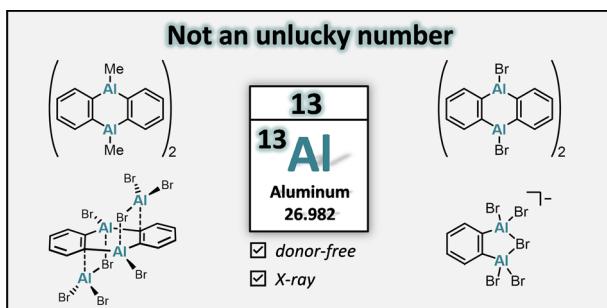
**P<sup>+</sup> addition and transfer involving a tetraphosphenium ion**

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



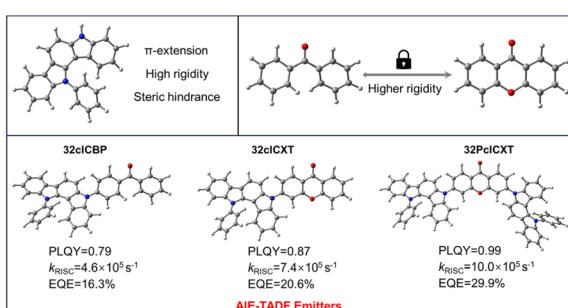
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**Donor-free 9,10-dihydro-9,10-dialuminaanthracenes**

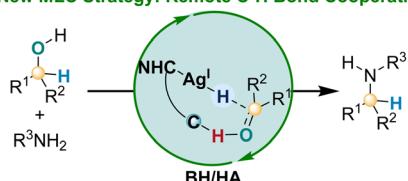
Paula L. Lückert, Jannik Gilmer, Alexander Virovets, Hans-Wolfram Lerner and Matthias Wagner\*

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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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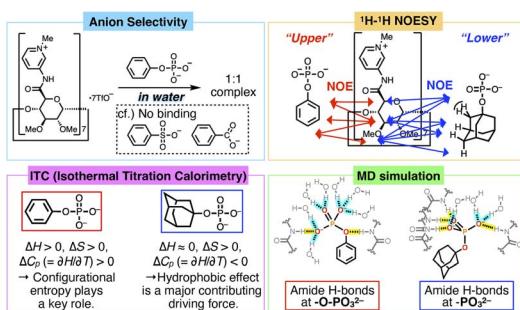
**New MLC Strategy: Remote C–H Bond Cooperation**

- 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

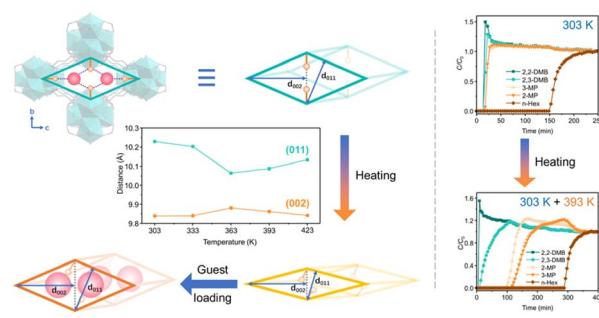


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**Synergistic global and local flexibilities in Zr-based metal–organic frameworks enable sequential sieving of hexane isomers**

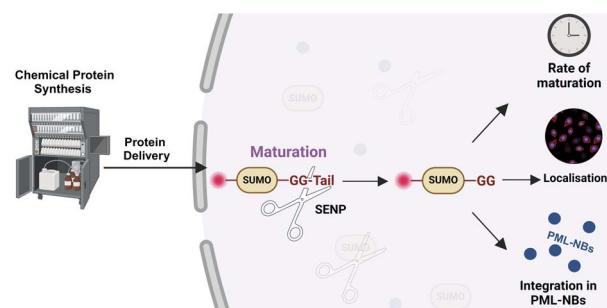
Rundao Chen, Jiaqi Li, Fang Zheng,\* Fangru Zhou, Bin Sheng, Baojian Liu, Qiwei Yang, Zhiguo Zhang, Qilong Ren and Zongbi Bao\*



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

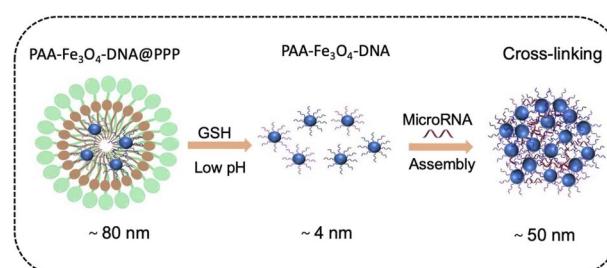
Dana Shkolnik, Subhasis Dey, Mahdi Hasan, Michael J. Matunis and Ashraf Brik\*



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

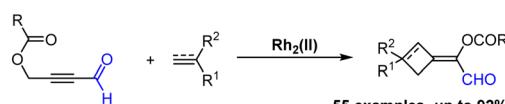
Yan Tan, Junren Wang, Qian Wan, Jinlong Yang, Jinkun Huang, Zijia Zhou, Haifeng Dong\* and Xueji Zhang\*



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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\*

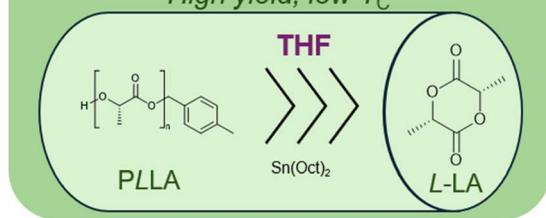


- Rh(II)-catalyzed 1,3-acyl migration of electronically deficient propargylic esters
- Tandem 1,3-acyl migration/intermolecular [2+2] cycloaddition
- Highly functionalized alkylidene cyclobutane/ene products
- Operationally simple, broad substrate scope



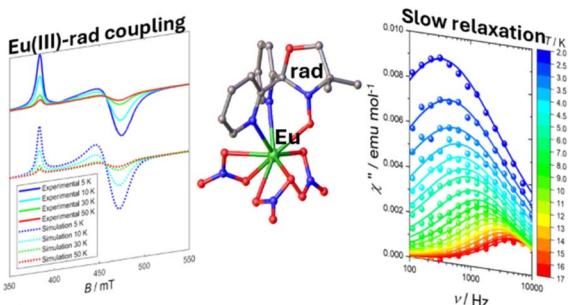
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**Continuous flow depolymerization***High yield, low  $T_C$* **Depolymerisation of poly(lactide) under continuous flow conditions**

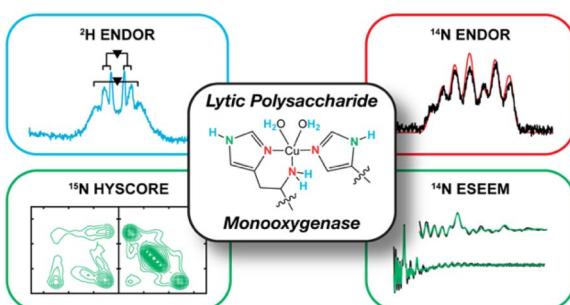
Sophie Ellis, Antoine Buchard\* and Tanja Junkers\*

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

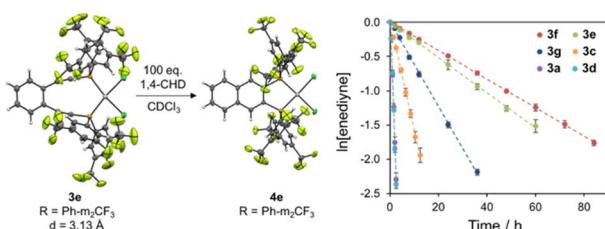
Lorenzo Sorace, Alexey A. Dmitriev, Mauro Perfetti\* and Kira E. Vostrikova\*

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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 HYSCORE spectroscopy**

Julia Haak, Ole Golten, Morten Sørlie, Vincent G. H. Eijssink and George E. Cutsail III\*

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**Pronounced electronic modulation of geometrically-regulated metallocenediyne cyclization**

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

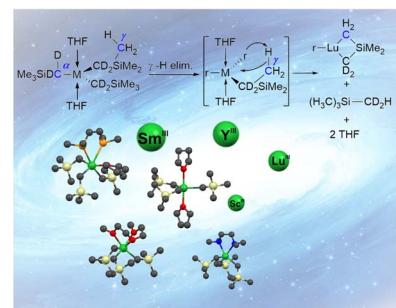


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**Stabilization of reactive rare earth alkyl complexes through mechanistic studies**

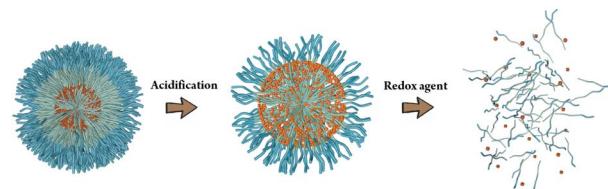
Elias Tanuhadi, Anna S. Bair, Mary Johnson, Philip Fontaine, Jerzy Klosin,\* Sudipta Pal and Polly L. Arnold\*



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

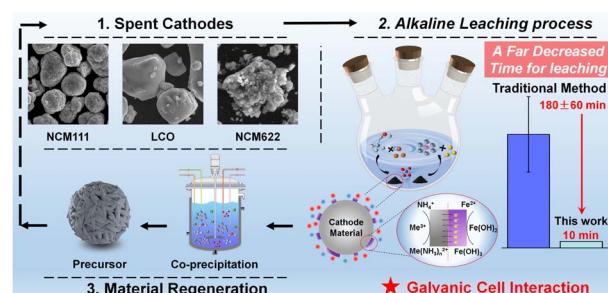
Yanting Gao, Fan Yang, Yufu Wang, Angus P. R. Johnston, Rebekah N. Duffin, Philip C. Andrews, Chris Ritchie\* and Georgina K. Such\*



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

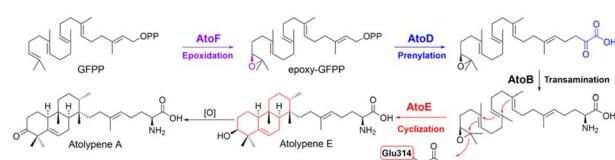
Long Ye, Zhilong Xu, Haiqiang Gong, Zhiming Xiao, Bao Zhang, Lei Ming and Xing Ou\*



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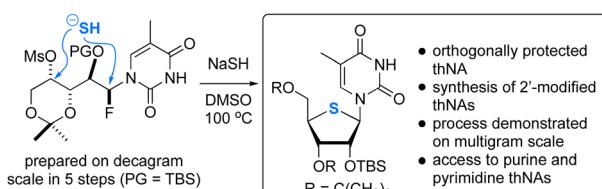
**Biosynthesis of a bacterial meroterpenoid reveals a non-canonical class II meroterpenoid cyclase**

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\*



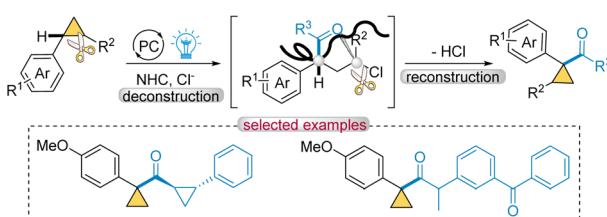
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**A flexible and scalable synthesis of 4'-thionucleosides**

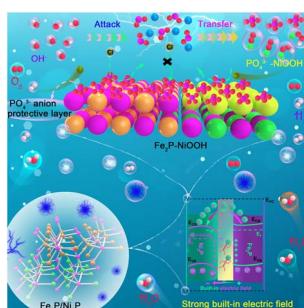
Callum Lucas, Ethan Fung, Matthew Nodwell, Steven Silverman, Bara Singh, Louis-Charles Campeau and Robert Britton\*

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

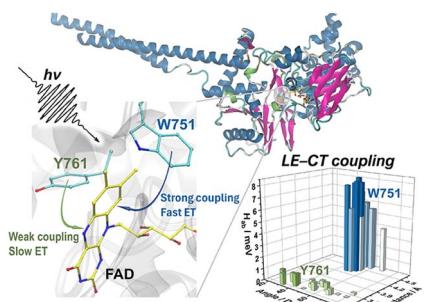
Fan Gao, Tian Wang and Xiaoyu Yan\*

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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\*

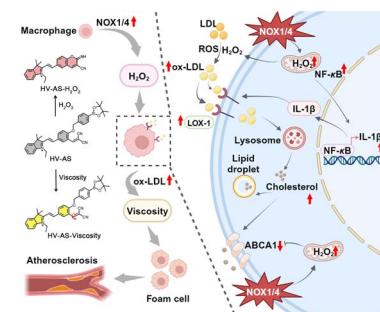


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**H<sub>2</sub>O<sub>2</sub> accumulation promoting internalization of ox-LDL in early atherosclerosis revealed via a synergistic dual-functional NIR fluorescence probe**

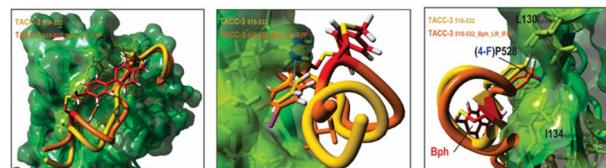
Hui Wang,\* Jingjing Guo, Tiancong Xiu, Yue Tang,\* Ping Li,\* Wei Zhang, Wen Zhang and Bo Tang\*



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

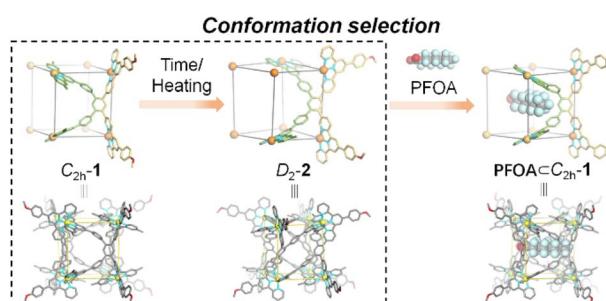
Diana Gimenez, Martin Walko, Jennifer A. Miles, Richard Bayliss,\* Megan H. Wright\* and Andrew J. Wilson\*



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**Dynamic selection in metallo-organic cube Cd<sup>II</sup>L<sub>4</sub> conformations induced by perfluorooctanoate encapsulation**

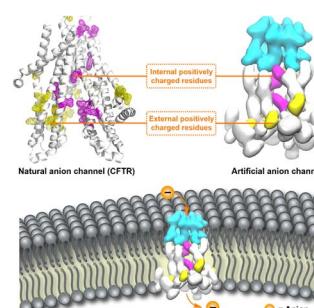
Yu-Qing Li, He Zhao, Ermeng Han, Zhiyuan Jiang,\* Qixia Bai, Yu-Ming Guan, Zhe Zhang, Tun Wu\* and Pingshan Wang\*



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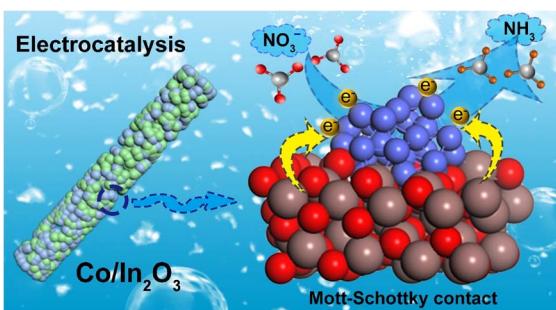
**Synthetic anion channels: achieving precise mimicry of the ion permeation pathway of CFTR in an artificial system**

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



## EDGE ARTICLES

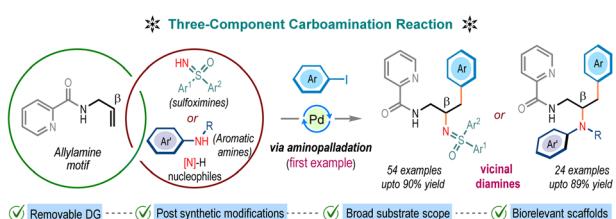
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## Enhanced electrocatalytic nitrate-to-ammonia performance from Mott–Schottky design to induce electron redistribution

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

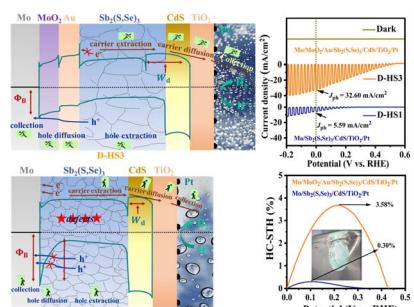
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## Regioselective intermolecular carboamination of allylamines *via* nucleopalladation: empowering three-component synthesis of vicinal diamines

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

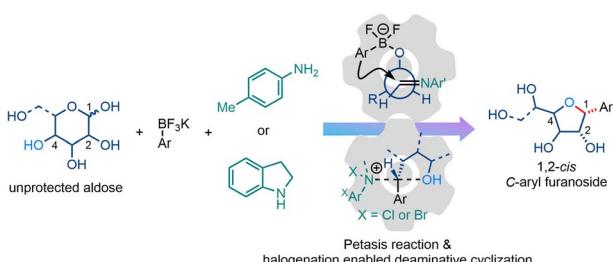
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## Dual back interface engineering optimized charge carrier dynamics in $\text{Sb}_2(\text{S},\text{Se})_3$ photocathodes for efficient solar hydrogen production

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\*

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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\*

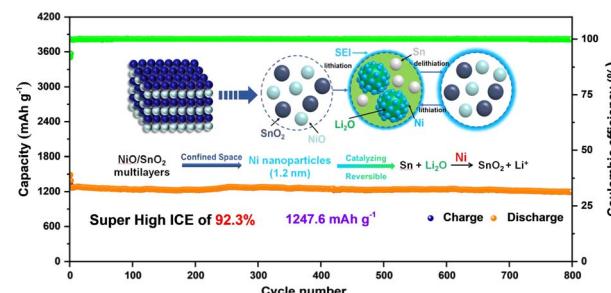


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**Spatially confined transition metals boost high initial coulombic efficiency in alloy anodes**

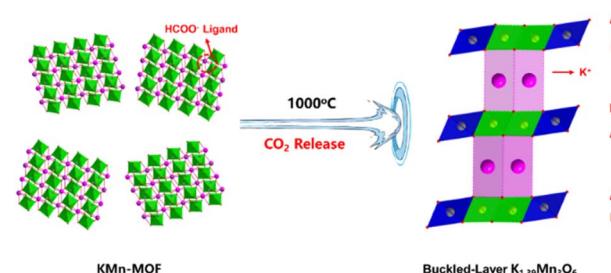
Haoyu Fu, Fangchao Gu, Yize Niu, Shuxuan Liao, Zeyuan Bu, Haonan Wang, Dong Yang, Xiaoshan Wang\* and Qiang Li\*



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**Buckled-layer  $K_{1.39}Mn_3O_6$ : a novel cathode for potassium-ion batteries**

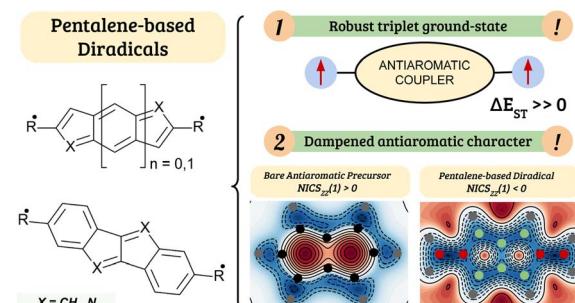
Ang Li, Ziqi Wang and Yunhua Xu\*



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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**

Chloé 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\*



## CORRECTIONS

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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\*

