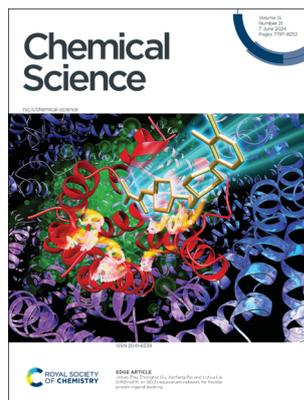


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(21) 7797–8252 (2024)



**Cover**  
See Won Bo Lee, Jonggeol Na *et al.*, pp. 7908–7925. Image reproduced by permission of Won Bo Lee from *Chem. Sci.*, 2024, 15, 7908.



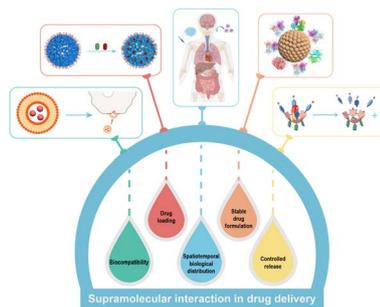
**Inside cover**  
See Jintao Zhu, Zhonghui Gu, Jianfeng Pei and Luhua Lai, pp. 7926–7942. Image reproduced by permission of Jintao Zhu, Zhonghui Gu, Jianfeng Pei and Luhua Lai from *Chem. Sci.*, 2024, 15, 7926.

## PERSPECTIVES

7811

### Supramolecular interaction in the action of drug delivery systems

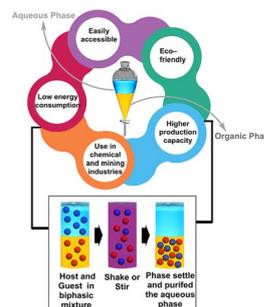
Wen-Chao Geng, Ze-Tao Jiang, Shi-Lin Chen and Dong-Sheng Guo\*



7824

### Supramolecular chemistry of liquid–liquid extraction

Sourav Pramanik, Abu S. M. Islam, Iti Ghosh and Pradyut Ghosh\*



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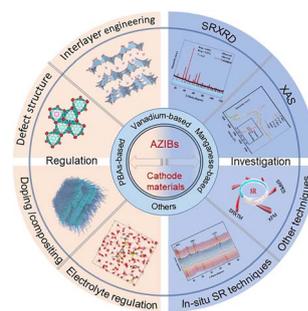
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## REVIEWS

7848

## Structure regulation and synchrotron radiation investigation of cathode materials for aqueous Zn-ion batteries

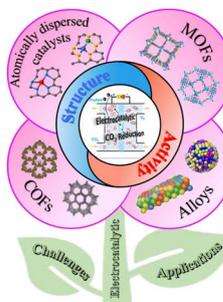
Shiqiang Wei, Yixiu Wang, Shuangming Chen\* and Li Song



7870

## Advances and challenges in the electrochemical reduction of carbon dioxide

Jingyi Han, Xue Bai, Xiaoqin Xu, Xue Bai, Anaer Husile, Siying Zhang, Luoluo Qi and Jingqi Guan\*

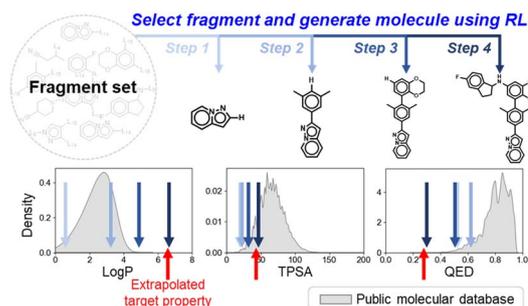


## EDGE ARTICLES

7908

## Materials discovery with extreme properties via reinforcement learning-guided combinatorial chemistry

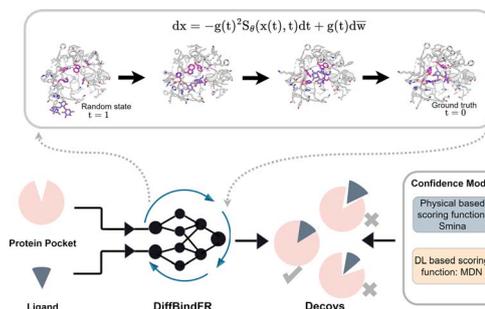
Hyunseung Kim, Haeyeon Choi, Dongju Kang, Won Bo Lee\* and Jonggeol Na\*



7926

## DiffBindFR: an SE(3) equivariant network for flexible protein–ligand docking

Jintao Zhu, Zhonghui Gu, Jianfeng Pei\* and Luhua Lai\*



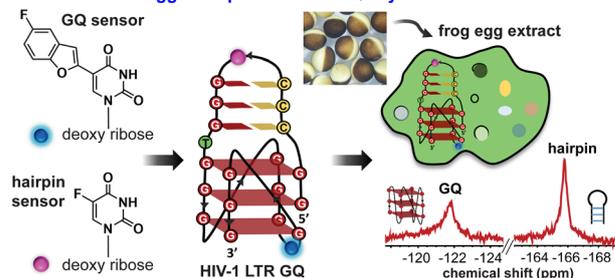


7982

### Structural elucidation of HIV-1 G-quadruplexes in a cellular environment and their ligand binding using responsive $^{19}\text{F}$ -labeled nucleoside probes

Sarupa Roy, Priyasha Majee, Sruthi Sudhakar, Satyajit Mishra, Jeet Kalia, P. I. Pradeepkumar\* and Seergazhi G. Srivatsan\*

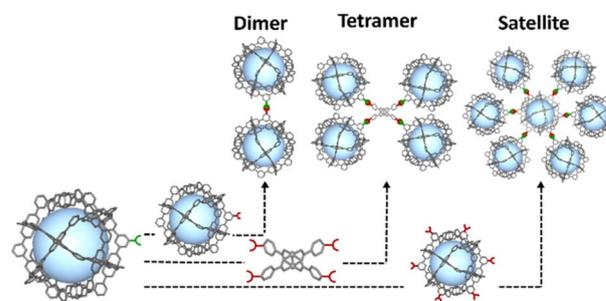
#### structure and druggable space of viral GQs by fluorescence and $^{19}\text{F}$ NMR



7992

### Giant oligomeric porous cage-based molecules

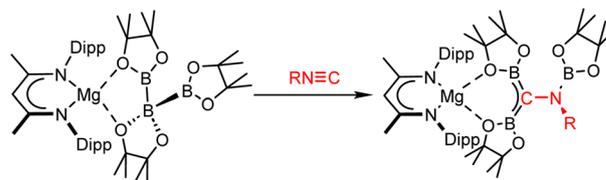
Alba Cortés-Martínez, Cornelia von Baeckmann, Laura Hernández-López, Arnau Carné-Sánchez\* and Daniel Maspoch\*



7999

### The borylamino-diborata-allyl anion

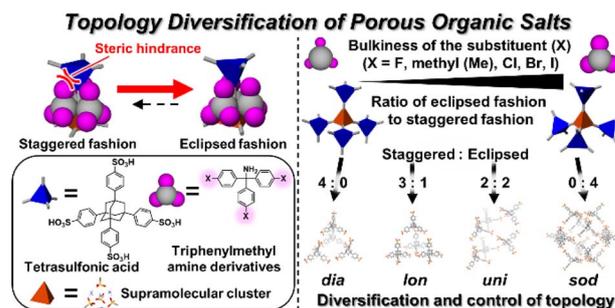
Henry T. W. Shere, Han-Ying Liu, Samuel E. Neale, Michael S. Hill,\* Mary F. Mahon and Claire L. McMullin\*



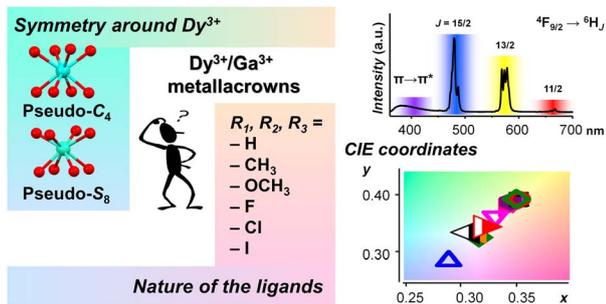
8008

### Network topology diversification of porous organic salts

Hiroi Sei, Kouki Oka, Yuta Hori, Yasuteru Shigeta and Norimitsu Tohnai\*



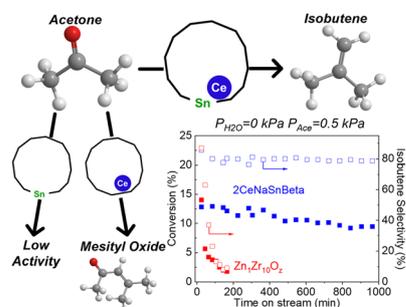
8019



### Tuning white light emission using single-component tetrachroic Dy<sup>3+</sup> metallacrowns: the role of chromophoric building blocks

Elvin V. Salerno, Svetlana V. Eliseeva,\* Stéphane Petoud\* and Vincent L. Pecoraro\*

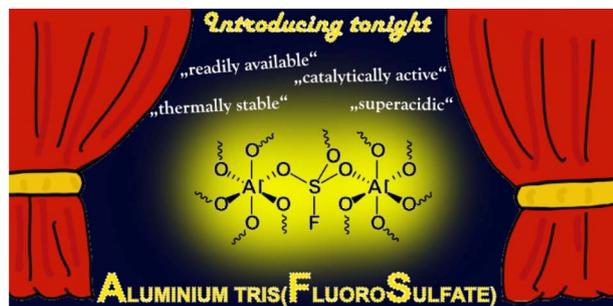
8031



### Confined dual Lewis acid centers for selective cascade C–C coupling and deoxygenation

Houqian Li, Jifeng Pang, Wenda Hu,\* Vanessa Caballero, Junming Sun,\* Mingwu Tan, Jian Zhi Hu, Yelin Ni and Yong Wang\*

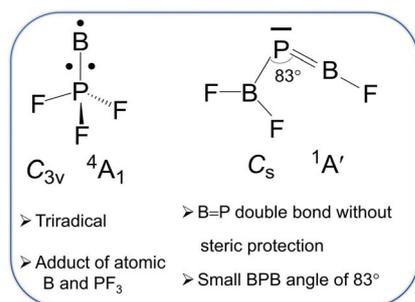
8038



### Introducing AFS ([Al(SO<sub>3</sub>F)<sub>3</sub>]<sub>x</sub>) – a thermally stable, readily available, and catalytically active solid Lewis superacid

Johanna Schögl, Ole Goldammer, Julia Bader, Franziska Emmerling and Sebastian Riedel\*

8045



### B=P double bonds relieved from steric encumbrance: matrix-isolation infrared spectroscopy of the phosphaborene F<sub>2</sub>B–P=BF and the triradical B=PF<sub>3</sub>

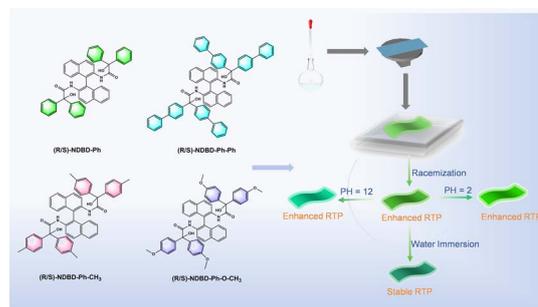
Mei Wen, Robert Medel, Pavel V. Zasimov, Carsten Müller and Sebastian Riedel\*



8052

### Employing racemization strategies to simultaneously enhance the quantum yield, lifetime, and water stability of room-temperature phosphorescent materials

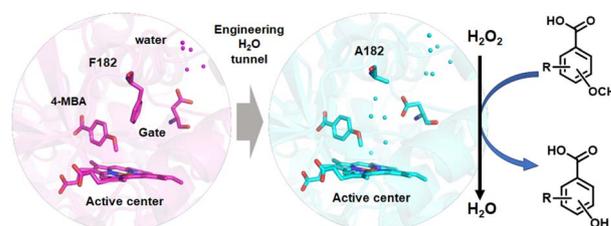
Zenggang Lin, Peng Zhang, Fuqiang Song, Yuzhu Yang, Xuan Miao and Weisheng Liu\*



8062

### Crucial gating residues govern the enhancement of peroxygenase activity in an engineered cytochrome P450 O-demethylase

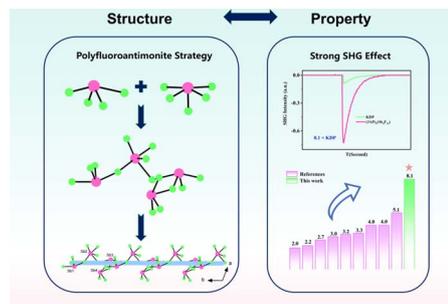
Panxia Zhao, Yiping Jiang, Qian Wang, Jie Chen, Fuquan Yao and Zhiqi Cong\*



8071

### [(C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>)<sub>2</sub>H](Sb<sub>4</sub>F<sub>13</sub>): a polyfluoroantimonite with a strong second harmonic generation effect

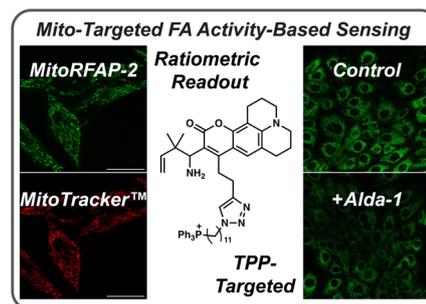
Jia-Hang Wu, Chun-Li Hu, Ya-Feng Li, Jiang-Gao Mao and Fang Kong\*



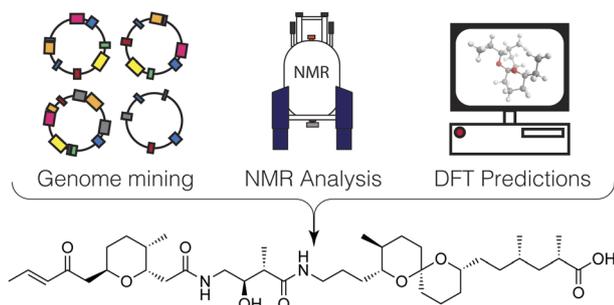
8080

### A mitochondrial-targeted activity-based sensing probe for ratiometric imaging of formaldehyde reveals key regulators of the mitochondrial one-carbon pool

Logan Tenney, Vanha N. Pham, Thomas F. Brewer and Christopher J. Chang\*



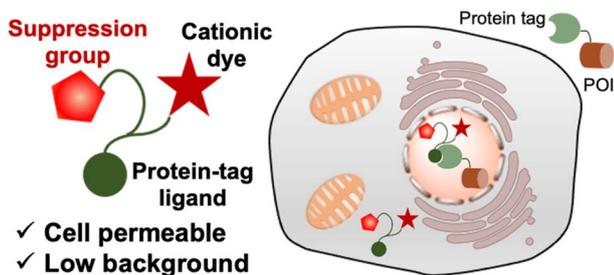
8089



### Discovery of a lagriamide polyketide by integrated genome mining, isotopic labeling, and untargeted metabolomics

Claire H. Fergusson, Julia Saulog, Bruno S. Paulo, Darryl M. Wilson, Dennis Y. Liu, Nicholas J. Morehouse, Samantha Waterworth, John Barkei, Christopher A. Gray, Jason C. Kwan, Alessandra S. Eustaquio\* and Roger G. Linington\*

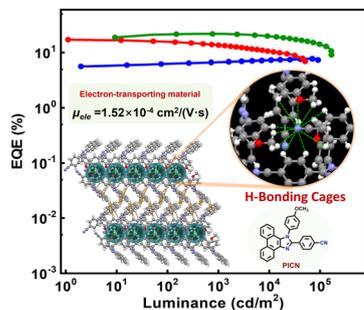
8097



### Bioisostere-conjugated fluorescent probes for live-cell protein imaging without non-specific organelle accumulation

Takuya Kamikawa, Akari Hashimoto, Nozomi Yamazaki, Junya Adachi, Ayami Matsushima, Kazuya Kikuchi\* and Yuichiro Hori\*

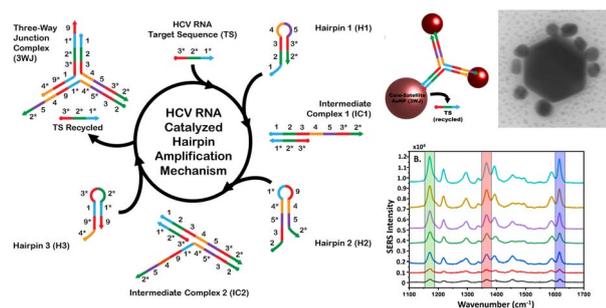
8106



### Improving electron transportation and operational lifetime of full color organic light emitting diodes through a "weak hydrogen bonding cage" structure

Huayi Zhou, Tengyue Li, Mingliang Xie, Yannan Zhou, Qikun Sun, Shi-Tong Zhang,\* Yujian Zhang,\* Wenjun Yang and Shanfeng Xue\*

8112



### DNA-directed formation of plasmonic core-satellite nanostructures for quantification of hepatitis C viral RNA

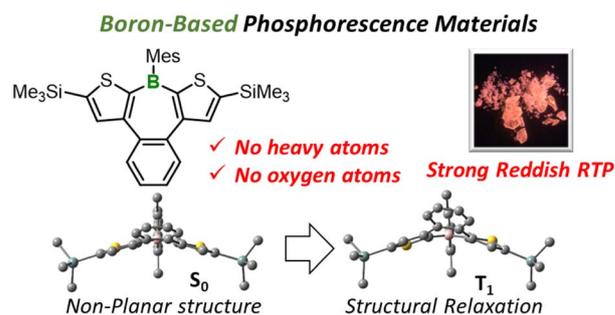
Siddhant Jaitpal, Ka Wai Ng, Angela Michelle San Juan, Cecilia Martinez, Christian Phillips, Sayantan Tripathy and Samuel Mabbott\*



8127

### Insights into mechanistic interpretation of crystalline-state reddish phosphorescence of non-planar $\pi$ -conjugated organoboron compounds

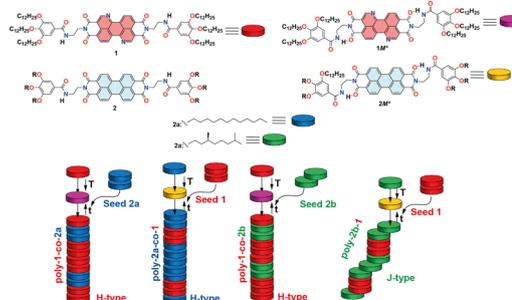
Yohei Adachi,\* Maho Kurihara, Kohei Yamada, Fuka Arai, Yuto Hattori, Keita Yamana, Riku Kawasaki and Joji Ohshita\*



8137

### Electronically and geometrically complementary perylenediimides for kinetically controlled supramolecular copolymers

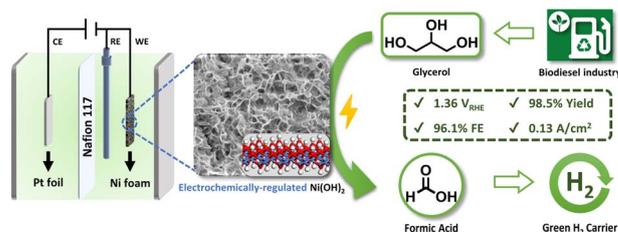
Alfonso J. Schwalb, Fátima García and Luis Sánchez\*



8145

### Redox regulation of Ni hydroxides with controllable phase composition towards biomass-derived polyol electro-refinery

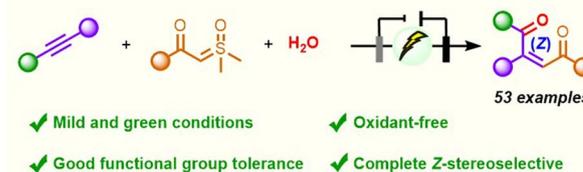
Zhuxin Gui, Yingshuai Jia, Xianping Liao, Tianlan Yan, Boxu Gao, Wenbiao Zhang, Li Chen, Qingsheng Gao,\* Yahong Zhang and Yi Tang\*



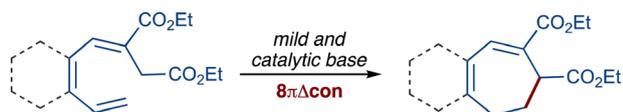
8156

### Electrochemical stereoselective synthesis of polysubstituted 1,4-dicarbonyl *Z*-alkenes via three-component coupling of sulfoxonium ylides and alkynes with water

Hao-Ran Li, Yi-An Ran, Yu-Yi Zhu, Weisi Guo, Shao-Fei Ni,\* Li-Rong Wen, Ming Li and Lin-Bao Zhang\*



8163

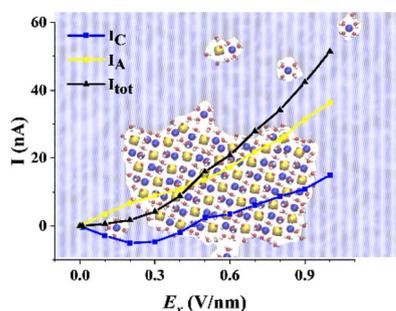


- **Mildest conditions** for electrocyclization of heptatrienyl anions
- First demonstration of **catalysis** and **organocatalysis**
- **Chain reaction** mechanism revealed

### Mild and catalytic electrocyclizations of heptatrienyl anions

Faizan Rasheed, Andrei Nikolaev, Anmol Dhesi, Tao Zeng, You Xuan Guo, Yarkali Krishna, Samira Komijani and Arturo Orellana\*

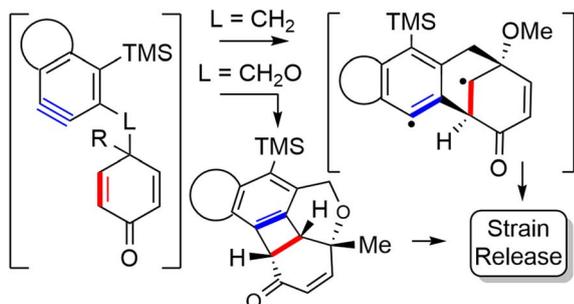
8170



### Formation of compounds with diverse polyelectrolyte morphologies and nonlinear ion conductance in a two-dimensional nanofluidic channel

Xiaoying Liang, Yanan Zhou, Weiduo Zhu, Wen Wu Xu, Joseph S. Francisco,\* Xiao Cheng Zeng\* and Wenhui Zhao\*

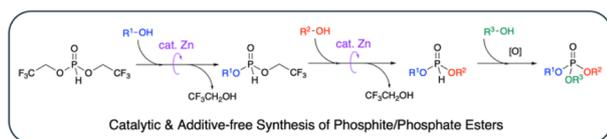
8181



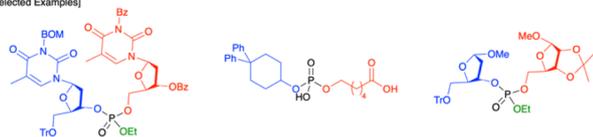
### Cascade reactions of HDDA-benzynes with tethered cyclohexadienones: strain-driven events originating from *ortho*-annulated benzocyclobutenes

Bhavani Shankar Chinta, Dorian S. Sneddon and Thomas R. Hoye\*

8190



[Selected Examples]



### A highly efficient catalytic method for the synthesis of phosphite diesters

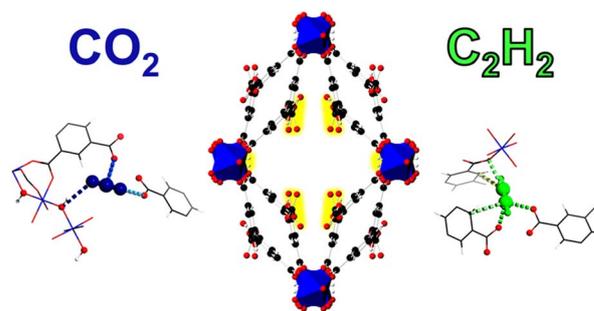
Yuki Saito, Soo Min Cho, Luca Alessandro Danieli, Akira Matsunaga and Shū Kobayashi\*



8197

### Binding of carbon dioxide and acetylene to free carboxylic acid sites in a metal–organic framework

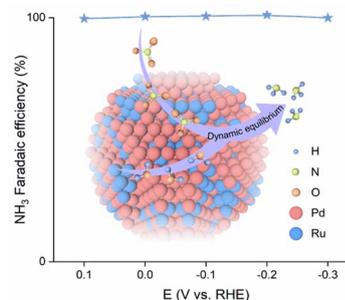
Christopher Marsh, Xue Han, Zhenzhong Lu, Ivan da Silva, Yongqiang Cheng, Luke L. Daemen, Sarah J. Day, Stephen P. Thompson, Anibal J. Ramirez-Cuesta, Sihai Yang\* and Martin Schröder\*



8204

### Alloying Pd with Ru enables electroreduction of nitrate to ammonia with ~100% faradaic efficiency over a wide potential window

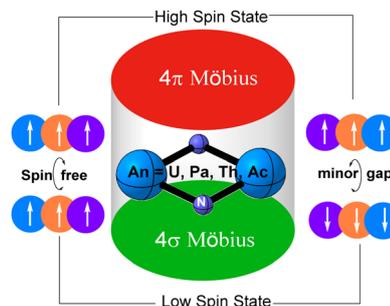
Yue Hu, Jiawei Liu, Wenyu Luo, Jinfeng Dong, Carmen Lee, Nan Zhang, Mengxin Chen, Yifan Xu, Dongshuang Wu, Mingsheng Zhang, Qiang Zhu, Erhai Hu, Dongsheng Geng,\* Lixiang Zhong\* and Qingyu Yan\*



8216

### Multiconfigurational actinide nitrides assisted by double Möbius aromaticity

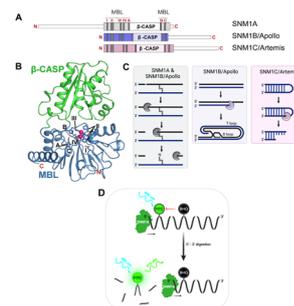
Xuhui Lin,\* Xiaoli Lu, Shenghui Tang, Wei Wu\* and Yirong Mo\*



8227

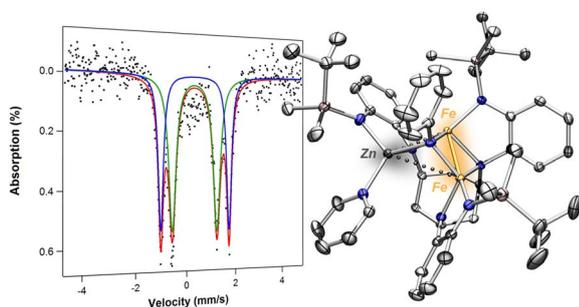
### Cell-active small molecule inhibitors validate the SNM1A DNA repair nuclease as a cancer target

Marcin Bielinski, Lucy R. Henderson, Yuliana Yosaatmadja, Lonnie P. Swift, Hannah T. Baddock, Matthew J. Bowen, Jürgen Brem, Philip S. Jones, Stuart P. McElroy, Angus Morrison, Michael Speake, Stan van Boeckel, Els van Doornmalen, Jan van Groningen, Helma van den Hurk, Opher Gileadi, Joseph A. Newman,\* Peter J. McHugh\* and Christopher J. Schofield\*



## EDGE ARTICLES

8242



### Cluster dynamics of heterometallic trinuclear clusters during ligand substitution, redox chemistry, and group transfer processes

Cristin E. Juda, Rex C. Handford, Amymarie K. Bartholomew, Tamara M. Powers, Nina X. Gu, Elisabeth Meyer, Nikolaj Roth, Yu-sheng Chen, Shao-Liang Zheng and Theodore A. Betley\*

## CORRECTION

8249

### Correction: Halogen-bonded charge-transfer co-crystal scintillators for high-resolution X-ray imaging

Yu-Hua Chen, Guo-Zhen Zhang, Fu-Hai Chen, Shu-Quan Zhang, Xin Fang,\* Hong-Ming Chen\* and Mei-Jin Lin\*

