

# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(27) 10251–10672 (2024)



**Cover**  
See Takeharu Yoshii, Hiroto Nishihara *et al.*, pp. 10350–10358. Image reproduced by permission of Takeharu Yoshii from *Chem. Sci.*, 2024, **15**, 10350.



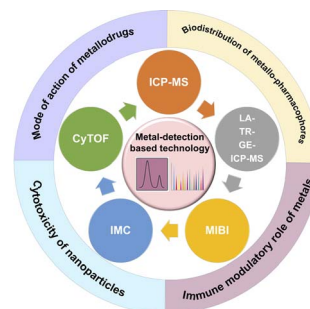
**Inside cover**  
See Marcus W. Drover *et al.*, pp. 10359–10365. Image reproduced by permission of Renee Man from *Chem. Sci.*, 2024, **15**, 10359.

## PERSPECTIVES

10264

### Metal-detection based techniques and their applications in metallobiology

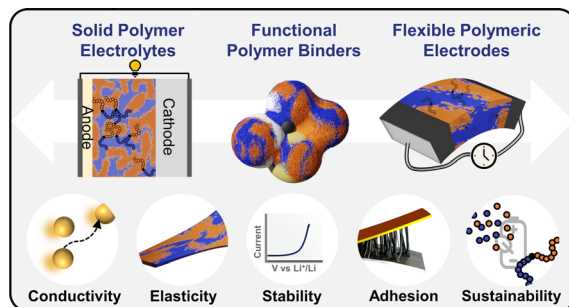
Ying Zhou,\* Hongyan Li,\* Eric Tse\* and Hongzhe Sun\*



10281

### Polymer design for solid-state batteries and wearable electronics

Kieran G. Stakem, Freddie J. Leslie and Georgina L. Gregory\*



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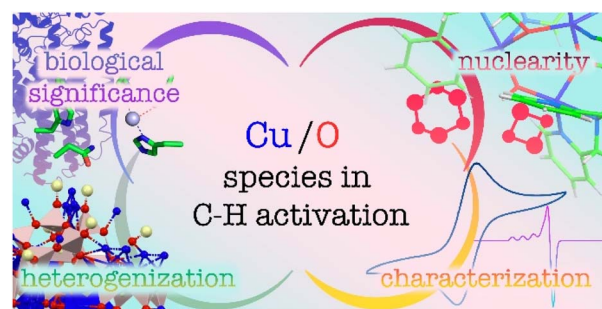
Fundamental questions  
Elemental answers

## REVIEW

10308

### Copper–oxygen adducts: new trends in characterization and properties towards C–H activation

Jonathan De Tovar, Rébecca Leblay, Yongxing Wang, Laurianne Wojcik, Aurore Thibon-Pourret, Marius Réglie, A. Jalila Simaan,\* Nicolas Le Poul\* and Catherine Belle\*

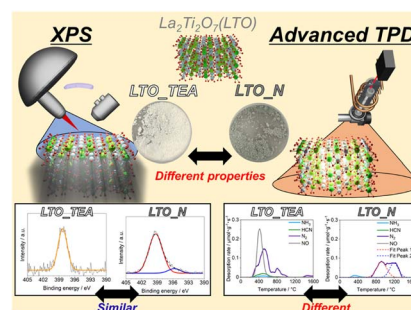


## EDGE ARTICLES

10350

### Unlocking the chemical environment of nitrogen in perovskite-type oxides

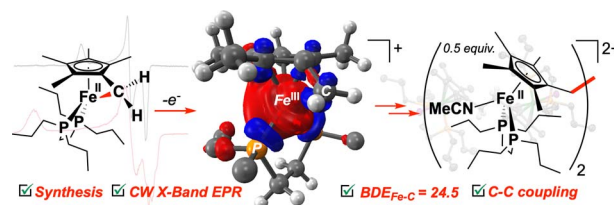
Shunsuke Shimizu, Takeharu Yoshii,\* Ginga Nishikawa, Jingwen Wang, Shu Yin, Eiichi Kobayashi and Hirotomo Nishihara\*



10359

### Oxidatively-induced C(sp<sup>3</sup>)–C(sp<sup>3</sup>) bond formation at a tucked-in iron(III) complex

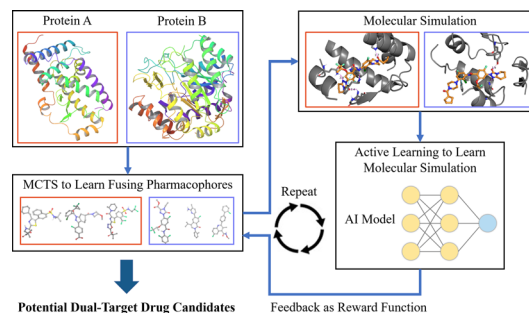
Joseph A. Zurakowski, Connor S. Durfy, Noah B. Stocck, Giovanni Fanchini and Marcus W. Drover\*



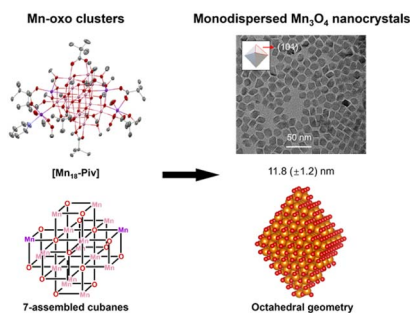
10366

### Structure-aware dual-target drug design through collaborative learning of pharmacophore combination and molecular simulation

Sheng Chen, Junjie Xie, Renlong Ye, David Daqiang Xu and Yuedong Yang\*



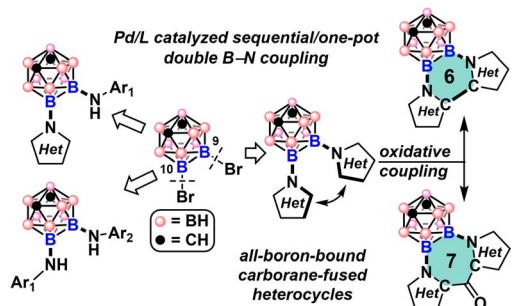
10381



### From cubane-assembled Mn-oxo clusters to monodispersed manganese oxide colloidal nanocrystals

Yan He, Yang Liu, Huijuan Zheng, Zhen Xiang, Zheng Zhou,\* Fengting Geng, Longlong Geng, Evgeny V. Dikarev\* and Haixiang Han\*

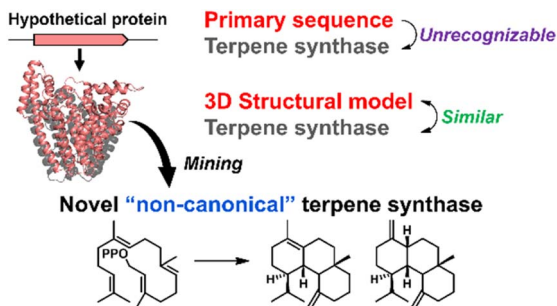
10392



### A Pd-catalyzed route to carborane-fused boron heterocycles

Mengjie Zhu, Puzhao Wang, Zhengqiu Wu, Yangfa Zhong, Laiman Su, Yuquan Xin, Alexander M. Spokoyny,\* Chao Zou\* and Xin Mu\*

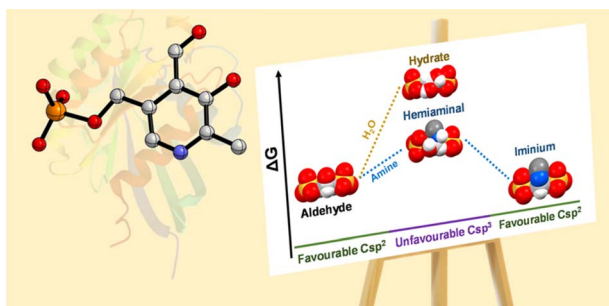
10402



### Structural-model-based genome mining can efficiently discover novel non-canonical terpene synthases hidden in genomes of diverse species

Tohru Abe, Haruna Shiratori, Kosuke Kashiwazaki, Kazuma Hiasa, Daijiro Ueda, Tohru Taniguchi, Hajime Sato,\* Takashi Abe\* and Tsutomu Sato\*

10408



### Key structural features to favour imines over hydrates in water: pyridoxal phosphate as a muse

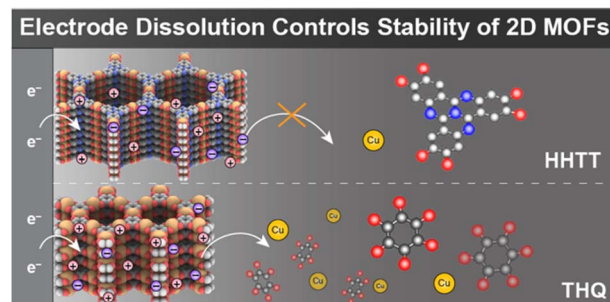
Ferran Esteve,\* Tanguy Rieu and Jean-Marie Lehn\*



10416

### Arresting dissolution of two-dimensional metal-organic frameworks enables long life in electrochemical devices

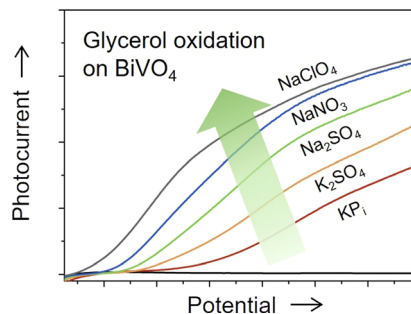
Gopi M. R. Dontireddy, Satya Prakash Suman, Jose L. Merino-Gardea, Tianyang Chen, Jin-Hu Dou\* and Harish Banda\*



10425

### Electrolyte selection toward efficient photoelectrochemical glycerol oxidation on BiVO<sub>4</sub>

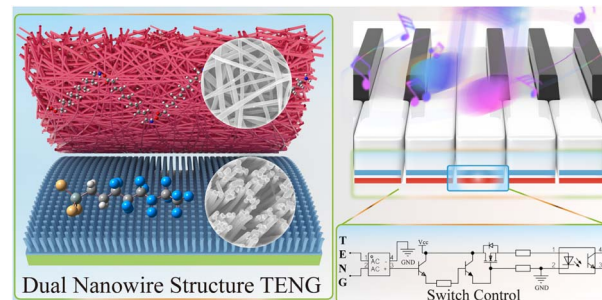
Heejung Kong, Siddharth Gupta, Andrés F. Pérez-Torres, Christian Höhn, Peter Bogdanoff, Matthew T. Mayer, Roel van de Krol, Marco Favaro\* and Fatwa F. Abdi\*



10436

### A high-performance triboelectric nanogenerator with dual nanostructure for remote control of switching circuit

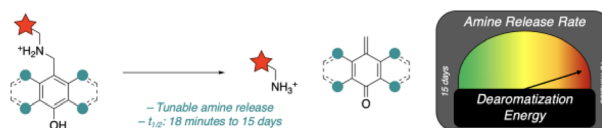
Yanhong Dong, Yange Feng\* and Daoai Wang\*



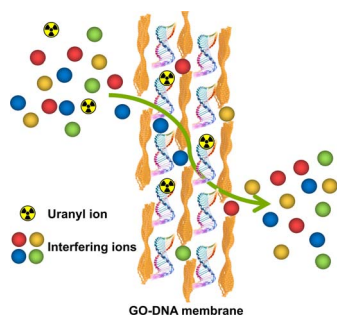
10448

### Controlling rates and reversibilities of elimination reactions of hydroxybenzylammoniums by tuning dearomatization energies

Zihuan Fu, Joseph W. Treacy, Brock M. Hosier, K. N. Houk\* and Heather D. Maynard\*



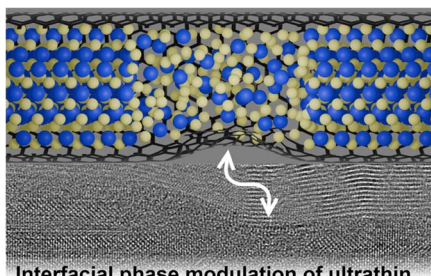
10455



### Designing biomimetic two-dimensional channels for uranium separation from seawater

Wenbin Liang, Xin Zhang, Liqin Wang, Chuanxi Wen, Longlong Tian,\* Zhan Li,\* Ximeng Chen and Wangsuo Wu

10464

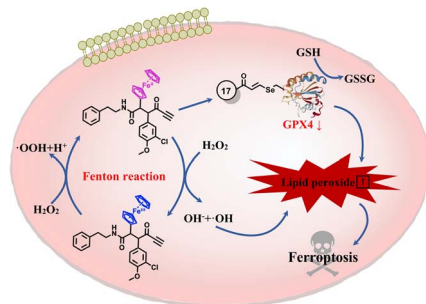


Interfacial phase modulation of ultrathin  $\text{Sb}_2\text{S}_3$  via nanotube encapsulation

### Encapsulation of crystalline and amorphous $\text{Sb}_2\text{S}_3$ within carbon and boron nitride nanotubes

Griffin M. Milligan, Dmitri Leo Mesoza Cordova, Ze-Fan Yao, Brian Y. Zhi, Lyndsey R. Scammell, Toshihiro Aoki and Maxx Arguilla\*

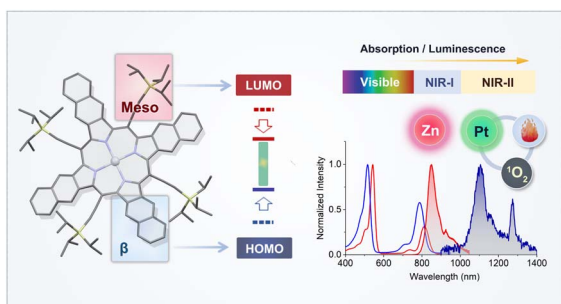
10477



### How does ferrocene correlate with ferroptosis? Multiple approaches to explore ferrocene-appended GPX4 inhibitors as anticancer agents

Wei Li, Jing Yu, Jing Wang, Xuejing Fan, Ximing Xu, Hui Wang, Ying Xiong, Xinyu Li, Xiaomin Zhang, Qianer Zhang, Xin Qi, Pascal Pigeon, Qing Gu, Julia Bruno-Colmenarez, Gérard Jaouen, Michael J. McGlinchey, Xue Qiu, Shu-Li You, Jing Li\* and Yong Wang\*

10491



### Synergistic *meso*- $\beta$ regulation of porphyrins: squeezing the band gap into the near-infrared I/II region

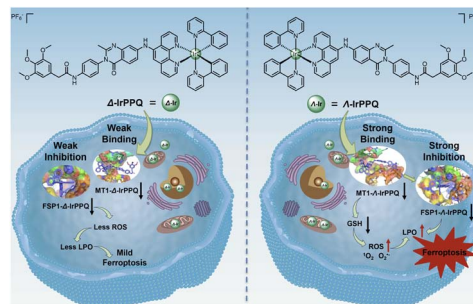
Chulin Qu, Xinxin Gong, Yufen Sun, Hu Gao, Fangjian Cai, Yue Zhao, Fan Wu\* and Zhen Shen\*



10499

## A $\Delta$ -Ir(III)-phenylquinazolinone complex enhances ferroptosis by selectively inhibiting metallothionein-1

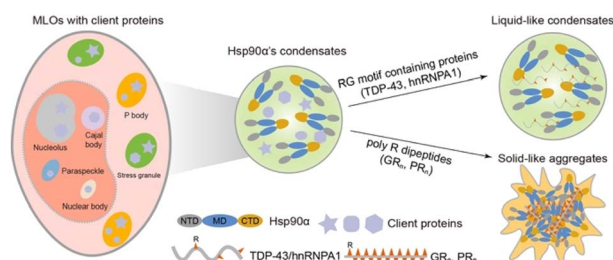
Lu Zhu, Xingyun Wang, Tian Tian, Yanyan Chen, Wenjing Du, Wei Wei,\* Jing Zhao,\* Zijian Guo and Xiuxiu Wang\*



10508

## Hsp90 $\alpha$ forms condensate engaging client proteins with RG motif repeats

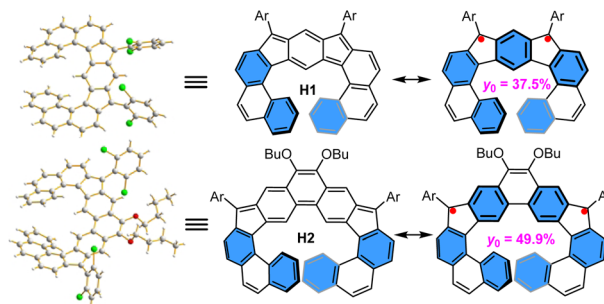
Jiaojiao Hu,\* Hui Dong, Yichen Li, Jing Gu, Liang Yang, Chenfang Si, Yaoyang Zhang, Tingting Li, Dan Li\* and Cong Liu\*



10519

## Helical polycyclic hydrocarbons with open-shell singlet ground states and ambipolar redox behaviors

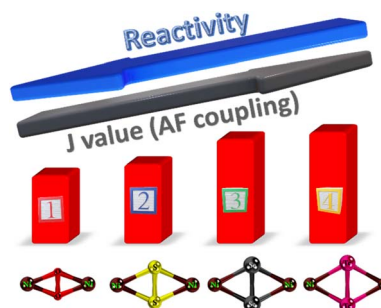
Qing Jiang,\* Hui Tang, Yuchen Peng, Zhenni Hu and Wangdong Zeng\*



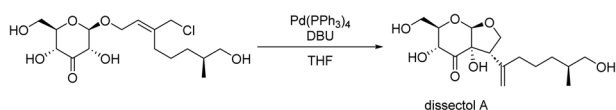
10529

## The interplay of covalency, cooperativity, and coupling strength in governing C–H bond activation in Ni<sub>2</sub>E<sub>2</sub> (E = O, S, Se, Te) complexes

Sunita Sharma, Bhawana Pandey and Gopalan Rajaraman\*



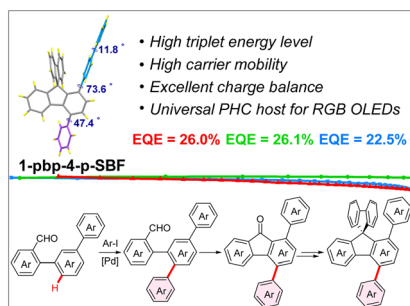
10541



### Total synthesis of dissectol A, using an enediolate-based Tsuji–Trost reaction

Ruben L. H. Andringa, Nittert Marinus, Daan V. Bunt, Elizabeth R. Haiderer, Robert B. Abramovitch, Christopher D. Brown, Kyu Y. Rhee, Martin D. Witte\* and Adriaan J. Minnaard\*

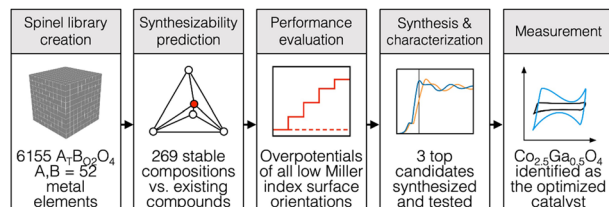
10547



### Crafting 1,4-diaryl spirobifluorene hosts in OLEDs via interannular C–H arylation: synergistic effects of molecular linearity and orthogonality

Qian Li, Zhiqian Yu, Qianhui Liu, Yusong Guo, Zhangyi Fu, Yudong Yang, Zhengyang Bin, Di Wu\* and Jingbo Lan\*

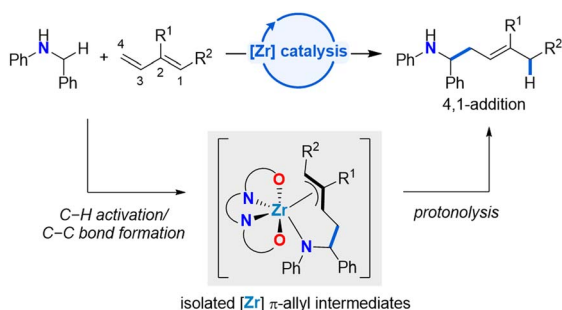
10556



### From computational screening to the synthesis of a promising OER catalyst

Sai Govind Hari Kumar, Carlota Bozal-Ginesta, Ning Wang, Jehad Abed, Chung Hsuan Shan, Zhenpeng Yao\* and Alan Aspuru-Guzik\*

10571



### Understanding mechanism driven regioselectivity in zirconium-catalysed hydroaminoalkylation: homoallylic amines from conjugated dienes

Erick Nuñez Bahena, Kimia Hosseini, Sheila Galván Curto and Laurel L. Schafer\*

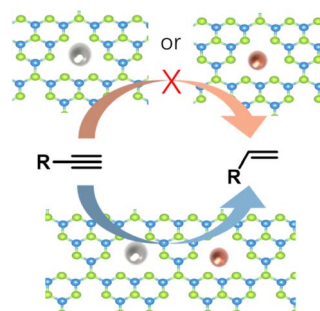




10577

### Expedient alkyne semi-hydrogenation by using a bimetallic AgCu–C<sub>3</sub>N<sub>4</sub> single atom catalyst

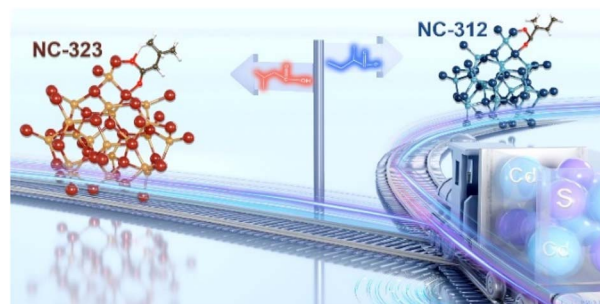
Jingting Song, Xiangbin Cai, Zhongxin Chen, Tie Wang, Shibo Xi, Qikun Hu, Ning Yan and Kian Ping Loh\*



10585

### Carboxylic acid isomer-directed synthesis of CdS nanocluster isomers

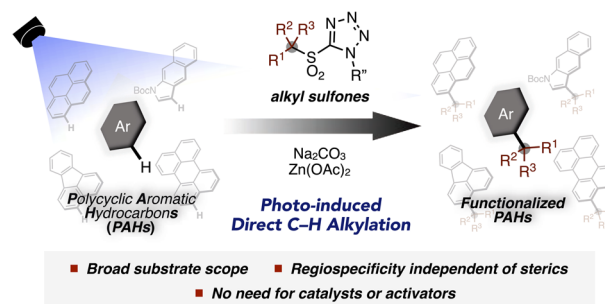
Jing Zhang,\* Yu Liu, Mingyang Liu, Zhenzhu Wang, Ting Qi, Mingming Zhang, Hao shi\* and Jun Song\*



10592

### Visible-light-induced direct C–H alkylation of polycyclic aromatic hydrocarbons with alkylsulfones

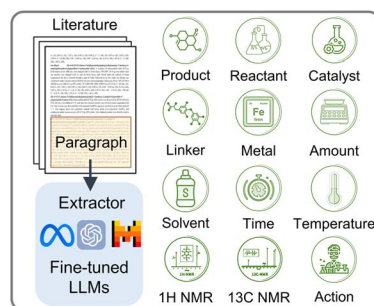
Motoo Ohtsuka, Koushik Ghosh, Jacky C.-H. Yim, Hikaru Sotome,\* Tsubasa Okamoto, Kayo Suda, Yasuhiro Kobori,\* Daisuke Yokogawa,\* Hiroshi Miyasaka,\* Cathleen M. Crudden\* and Masakazu Nambo\*



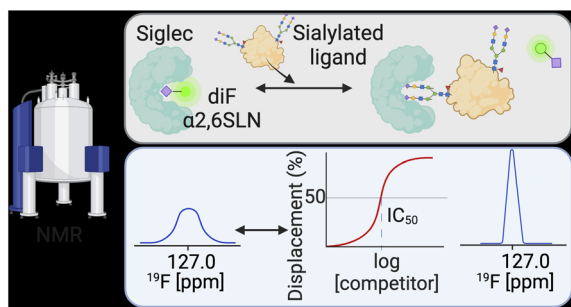
10600

### Fine-tuning large language models for chemical text mining

Wei Zhang, Qinggong Wang, Xiangtai Kong, Jiacheng Xiong, Shengkun Ni, Duanhua Cao, Buying Niu, Mangan Chen, Yameng Li, Runze Zhang, Yitian Wang, Lehan Zhang, Xutong Li, Zhaoping Xiong, Qian Shi, Ziming Huang, Zunyun Fu\* and Mingyue Zheng\*



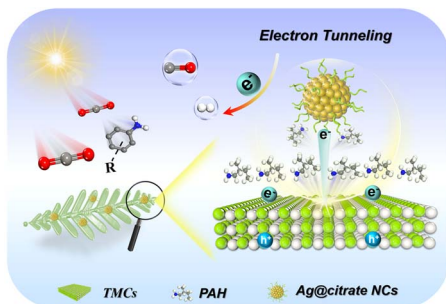
10612



### Quantifying Siglec-sialylated ligand interactions: a versatile $^{19}\text{F}$ -T<sub>2</sub> CPMG filtered competitive NMR displacement assay

Unai Atxabal, Andrea Fernández, María Jesús Moure, Klaudia Sobczak, Corwin Nycholat, Verónica Almeida-Marrero, Iker Oyenarte, James C. Paulson, Andrés de la Escosura, Tomás Torres, Niels C. Reichardt, Jesús Jiménez-Barbero\* and June Ereño-Orbea\*

10625



### Photocatalyst tunneling triggering CO<sub>2</sub> photocatalysis

Xian Yan, Meng Yuan, Ya-Long Yuan, Peng Su, Qing Chen and Fang-Xing Xiao\*

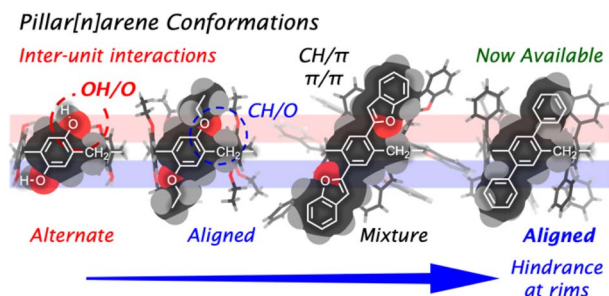
10638



### Discovery of molybdenum based nitrogen fixation catalysts with genetic algorithms

Magnus Strandgaard, Julius Seumer and Jan H. Jensen\*

10651



### Pillar[5]arenes decorated with six-membered-ring aromatics at all the substitution positions

Tomoya Kaneda, Kenichi Kato,\* Shunsuke Ohtani and Tomoki Ogoshi\*

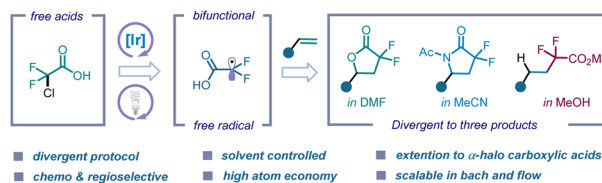


## EDGE ARTICLES

10659

**Divergent functionalization of alkenes enabled by photoredox activation of CDFA and  $\alpha$ -halo carboxylic acids**

Rahul Giri, Egor Zhilin and Dmitry Katayev\*



## CORRECTIONS

10668

**Correction: Phosphorescent [3 + 2 + 1] coordinated Ir(III) cyano complexes for achieving efficient phosphors and their application in OLED devices**

Yuan Wu, Chen Yang,\* Jie Liu, Meng Zhang, Weiqiang Liu, Wansi Li, Chengcheng Wu, Gang Cheng,\* Qingdan Yang,\* Guodan Wei\* and Chi-Ming Che

10669

**Correction: Neutral inverse-sandwich rare-earth metal complexes of the benzene tetraanion**

Yi Wang, Yurou Zhang, Jiefeng Liang, Bowen Tan, Chong Deng and Wenliang Huang\*

