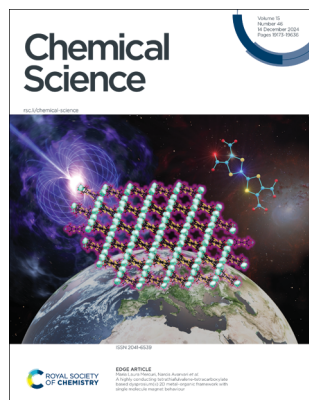


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(46) 19173–19636 (2024)



### Cover

See Maria Laura Mercuri, Narcis Avarvari *et al.*, pp. 19247–19263. Image reproduced by permission of F. Manna, M. Oggianu, M.L. Mercuri and N. Avarvari from *Chem. Sci.*, 2024, **15**, 19247.



### Inside cover

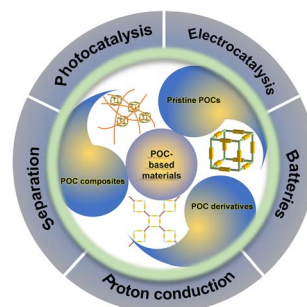
See Guido H. Clever *et al.*, pp. 19264–19272. Image reproduced by permission of Guido H. Clever from *Chem. Sci.*, 2024, **15**, 19264. Image created by Sabine König using Adobe Firefly.

## PERSPECTIVES

19188

### Recent advances in porous organic cages for energy applications

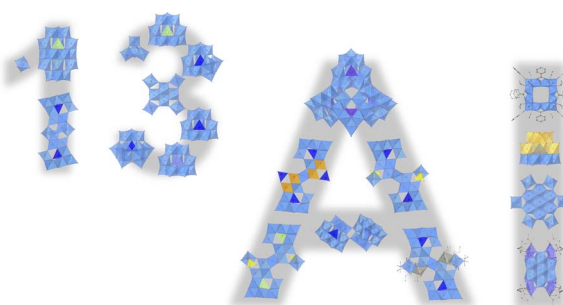
Chao Liu, Zhixuan Wang, Hailong Wang\* and Jianzhuang Jiang\*



19212

### Cationic Al oxo-hydroxide clusters: syntheses, molecular structures, and functional applications

Naoki Ogiwara, Wei Zhou and Sayaka Uchida\*



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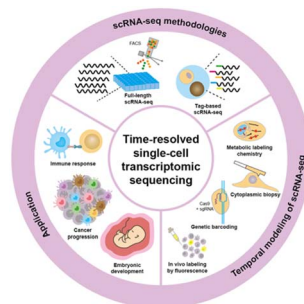
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## REVIEW

19225

## Time-resolved single-cell transcriptomic sequencing

Xing Xu, Qianxi Wen, Tianchen Lan, Liuqing Zeng, Yonghao Zeng, Shiyan Lin, Minghao Qiu, Xing Na and Chaoyong Yang\*

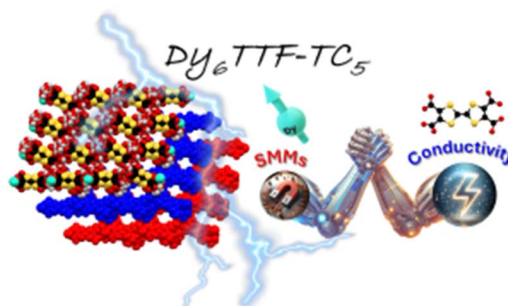


## EDGE ARTICLES

19247

**A highly conducting tetrathiafulvalene-tetracarboxylate based dysprosium(III) 2D metal-organic framework with single molecule magnet behaviour**

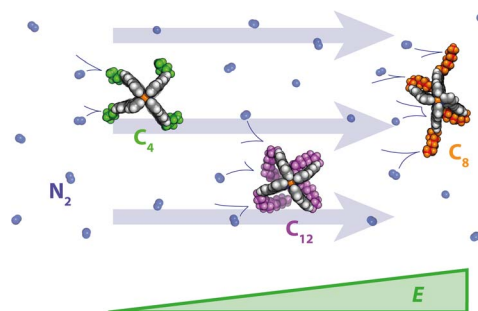
Fabio Manna, Mariangela Oggianu, Pascale Auban-Senzier, Ghenadie Novitchi, Enric Canadell, Maria Laura Mercuri\* and Narcis Avarvari\*



19264

**London dispersion driven compaction of coordination cages in the gas-phase – a combined ion mobility and theoretical study**

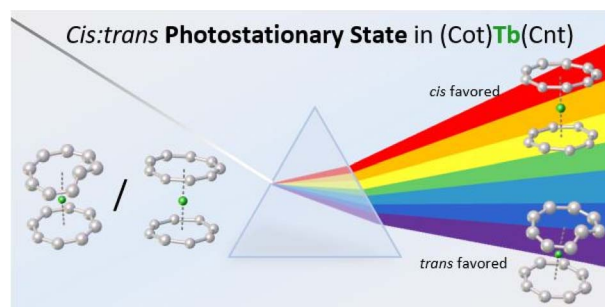
Christoph Drechsler, Ananya Baksi, André Platzek, Mert Acar, Julian J. Holstein, Christopher J. Stein and Guido H. Clever\*



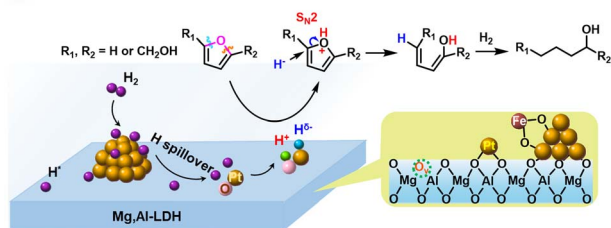
19273

**The photo-isomerization of the cyclononatetraenyl ligand and related rare earth complexes**

Lucie Pedussaut, Nolwenn Mahieu, Camille Chartier, Thayalan Rajeshkumar, Maxime Tricoire, Iskander Douair, Nicolas Casaretto, Laurent Maron, Grégory Danoun\* and Grégory Nocton\*



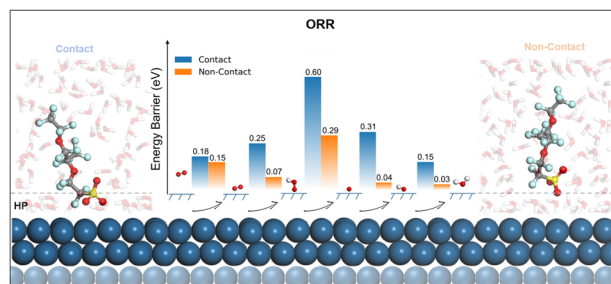
19283



### Selective hydrogenolysis of the Csp<sup>2</sup>–O bond in the furan ring using hydride–proton pairs derived from hydrogen spillover

Fangfang Peng, Bin Zhang, Runyao Zhao, Shiqiang Liu, Yuxuan Wu, Shaojun Xu, Luke L. Keenan, Huizhen Liu, Qingli Qian, Tianbin Wu, Haijun Yang, Zhimin Liu, Jikun Li,\* Bingfeng Chen,\* Xinchun Kang\* and Buxing Han\*

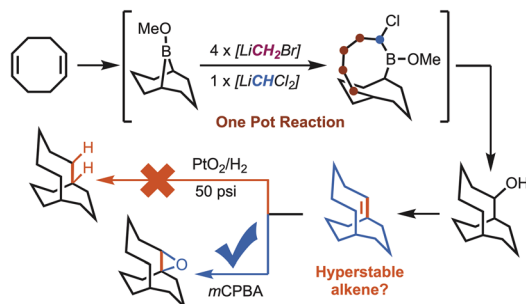
19290



### Influence of the Pt/ionomer/water interface on the oxygen reduction reaction: insights into the micro-three-phase interface

Shangkun Jiang, Qiong Xiang, Zhuoyang Xie, Na Yang, Jiawei Liu, Li Li\* and Zidong Wei\*

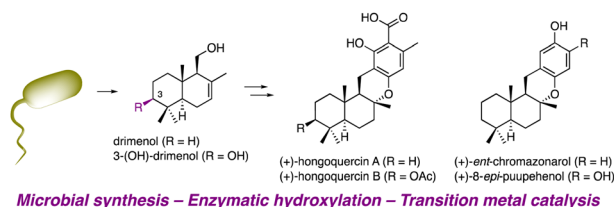
19299



### Hyperstable alkenes: are they remarkably unreactive?

Matthew D. Summersgill, Lawrence R. Gahan, Sharon Chow, Gregory K. Pierens, Paul V. Bernhardt, Elizabeth H. Krenske and Craig M. Williams\*

19307



### Unified enantiospecific synthesis of drimane meroterpenoids enabled by enzyme catalysis and transition metal catalysis

Yipeng You, Xue-Jie Zhang, Wen Xiao, Thittaya Kunthich, Zheng Xiang\* and Chen Xu\*

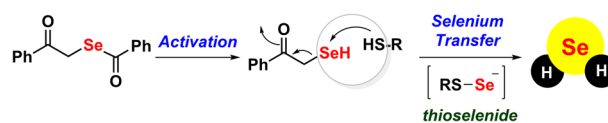


## EDGE ARTICLES

19315

**Phenacylselenoesters allow facile selenium transfer and hydrogen selenide generation**

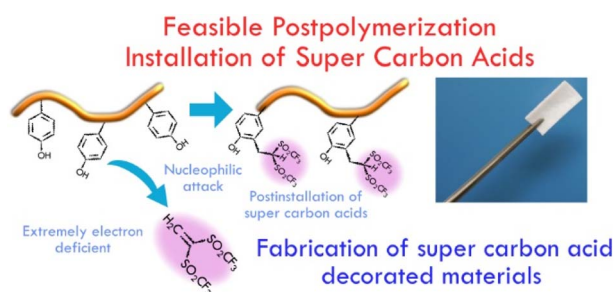
Utsav Dey Sarkar, Mahima Rana and Harinath Chakrapani\*



19322

**Installation of superacidic carbon acid moieties into polymer materials via post-polymerization modification**

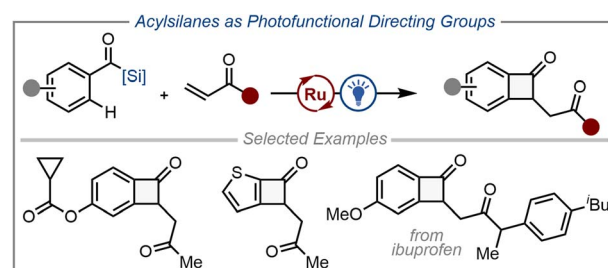
Ryohei Kakuchi,\* Takuma Oguchi, Minoru Kuroiwa, Yu Hirashima, Masaaki Omichi, Noriaki Seko\* and Hikaru Yanai\*



19328

**Benzocyclobutenone synthesis exploiting acylsilanes as photofunctional directing groups**

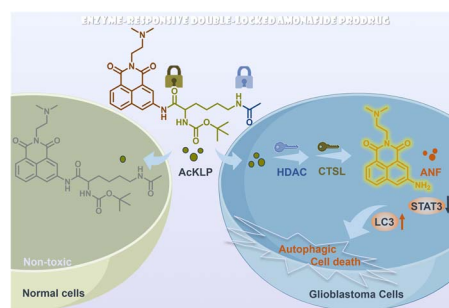
Rowan L. Pilkington, Hannah J. Ross, Liselle Atkin and Daniel L. Priebbenow\*



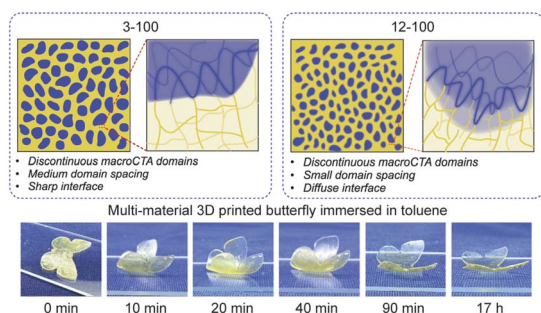
19336

**An enzyme-responsive double-locked amonafide prodrug for the treatment of glioblastoma with minimal side effects**

Wei Cheng, Yanli Yang, Bo Zhang,\* Chen-Wen Shao, Wei Chen, Ruimin Xia, Wenwei Sun, Xiubo Zhao, Bing Zhang, Xiangjie Luo,\* Tony D. James\* and Yong Qian\*



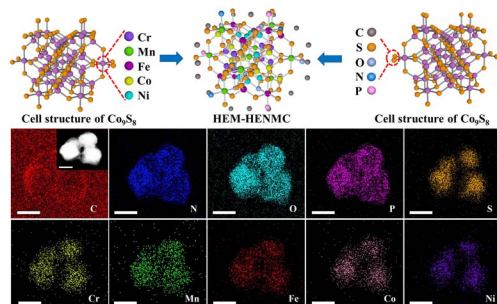
19345



### Nanostructure design of 3D printed materials through macromolecular architecture

Di Wu, Vaibhav Dev, Valentin A. Bobrin, Kenny Lee and Cyrille Boyer\*

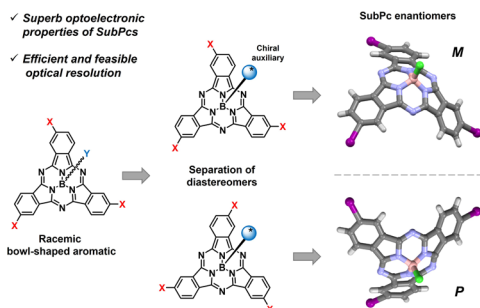
19359



### A high entropy metallic–high entropy nonmetallic community as a high performance electrocatalyst for the oxygen evolution reaction and oxygen reduction reaction

Chunyan Zhang, Hang Li, Mengfei Su, Shengfa Li, Feng Gao\* and Qingyi Lu\*

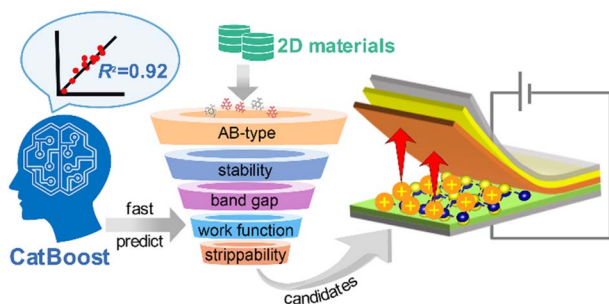
19369



### Optical resolution via chiral auxiliaries of curved subphthalocyanine aromatics

Giulia Lavarda, Lara Tejerina, Tomás Torres\* and M. Victoria Martínez-Díaz\*

19375



### Machine learning-assisted high-throughput screening of transparent organic light-emitting diode anode materials

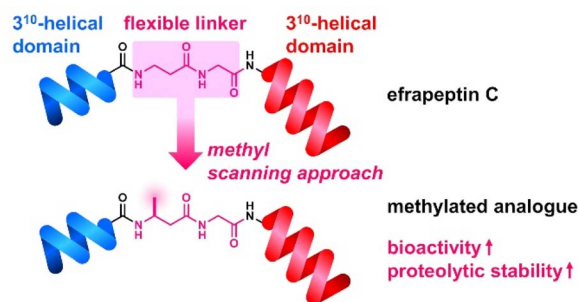
Liying Cui, Qing Li, Yanchang Zhang, Jiao Zhang, Zhe Wang, Jiankang Chen and Bing Zheng\*



19390

### Methyl scanning approach for enhancing the biological activity of the linear peptidic natural product, efrapeptin C

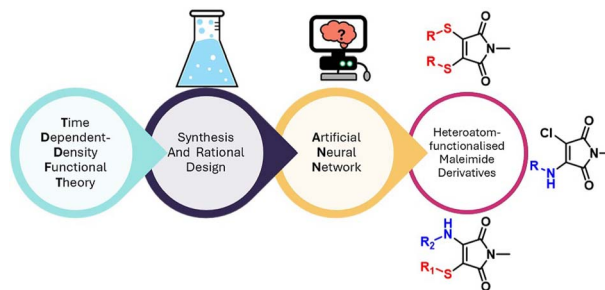
Yuanqi Lin, Hiroaki Itoh, Shingo Dan and Masayuki Inoue\*



19400

### Integrated computational and experimental design of fluorescent heteroatom-functionalised maleimide derivatives

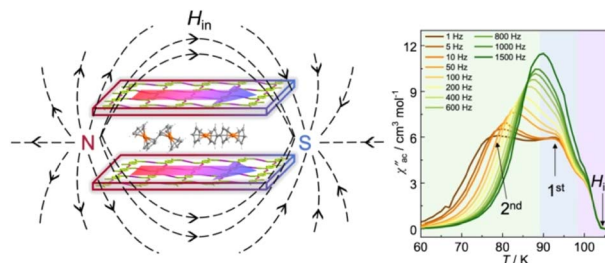
Jake E. Barker, Gareth W. Richings, Yujie Xie, Julia Y. Rho, Calum T. J. Ferguson, Rachel K. O'Reilly\* and Scott Habershon\*



19411

### Dynamic spin reordering in a hybrid layered ferrimagnet with intercalated biferrocenium radicals

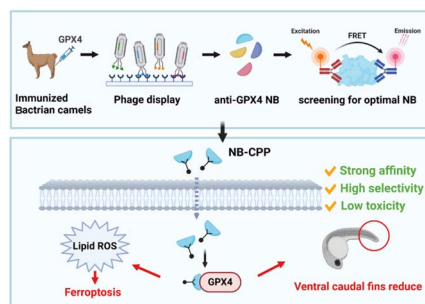
Qingxin Liu, Wataru Kosaka and Hitoshi Miyasaka\*



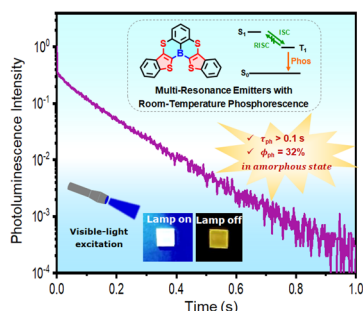
19420

### A potent and selective anti-glutathione peroxidase 4 nanobody as a ferroptosis inducer

Xinyu Li, Yaru Li, Aowei Xie, Fenglin Chen, Jing Wang, Jianfeng Zhou, Ximing Xu, Zhenlin Xu,\* Yong Wang\* and Xue Qiu\*



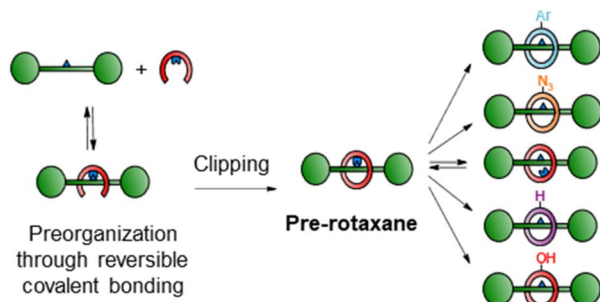
19432



### Multi-resonance emitters with room-temperature phosphorescence in amorphous state and excited by visible light

Baoyun Du, Yuliang Wu, Xingdong Wang, Hongkun Tian, Shiyang Shao\* and Lixiang Wang\*

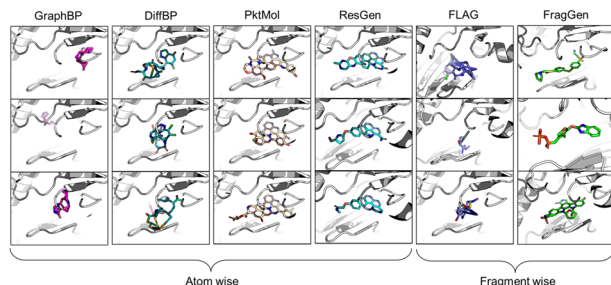
19443



### Boronic ester-templated pre-rotaxanes as versatile intermediates for rotaxane *endo*-functionalisation

Jingjing Yu, Marius Gaedke, Satyajit Das, Daniel L. Stares, Christoph A. Schalley and Fredrik Schaufelberger\*

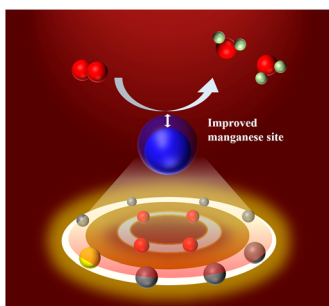
19452



### FragGen: towards 3D geometry reliable fragment-based molecular generation

Odin Zhang, Yufei Huang, Shichen Cheng, Mengyao Yu, Xujun Zhang, Haitao Lin, Yundian Zeng, Mingyang Wang, Zhenxing Wu, Huifeng Zhao, Zaixi Zhang, Chenqing Hua, Yu Kang, Sunliang Cui,\* Peichen Pan,\* Chang-Yu Hsieh\* and Tingjun Hou\*

19466



### Double coordination shell modulation of nitrogen-free atomic manganese sites for enhancing oxygen reduction performance

Xue Bai, Yin Wang, Jingyi Han, Siyu Chen, Xiaodi Niu\* and Jingqi Guan\*

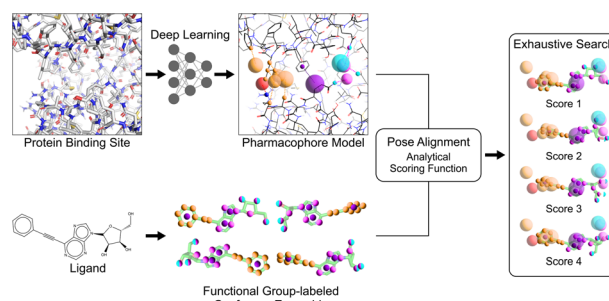


## EDGE ARTICLES

19473

**PharmacoNet: deep learning-guided pharmacophore modeling for ultra-large-scale virtual screening**

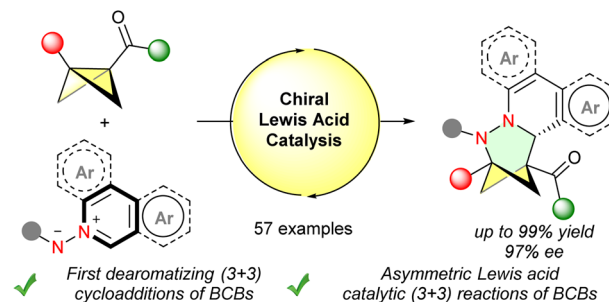
Seonghwan Seo and Woo Youn Kim\*



19488

**Enantioselective dearomative formal (3+3) cycloadditions of bicyclobutanes with aromatic azomethine imines: access to fused 2,3-diazabicyclo [3.1.1]heptanes**

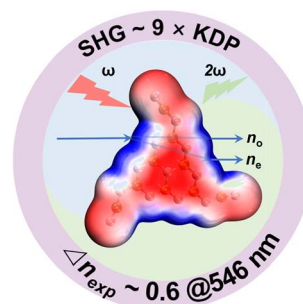
Xue-Chun Yang, Feng Wu, Wen-Biao Wu, Xu Zhang and Jian-Jun Feng\*



19496

**Large second harmonic generation and birefringence from extended octupolar  $\pi$ -conjugated structures**

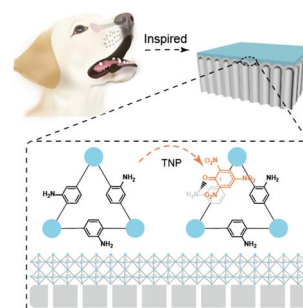
Danyang Dou, Bingbing Zhang, Daqing Yang and Ying Wang\*



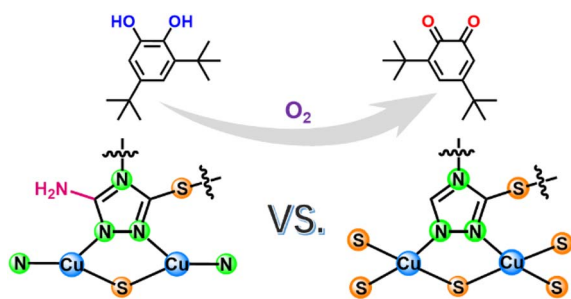
19504

**An ultrasensitive 2,4,6-trinitrophenol nanofluidic sensor inspired by olfactory sensory neurons in sniffer dogs**

Xin Li, Zhanfang Liu, Linsen Yang, Shengyang Zhou, Yongchao Qian, Yuge Wu, Zidi Yan, Zehua Zhang, Tingyang Li, Qingchen Wang, Congcong Zhu,\* Xiang-Yu Kong and Liping Wen\*



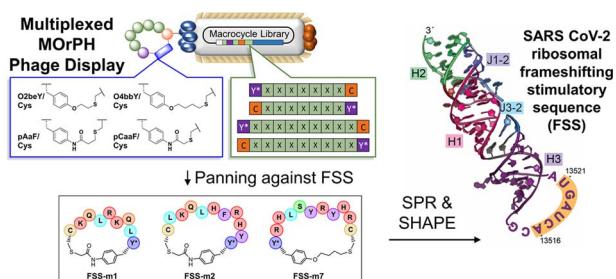
19513



### Steering N/S coordination number to accelerate catecholase-like catalysis over low-coordinated Cu site

Meng Yuan, Nannan Xia, Ziheng Huang, Chaofeng Huang, Xun Hu\* and Fei He\*

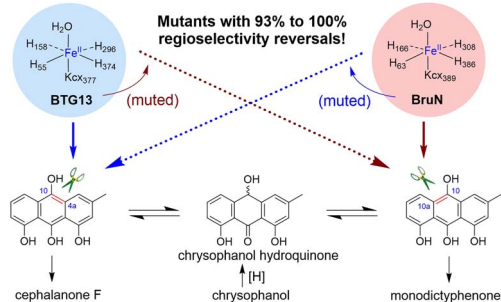
19520



### Cyclic peptides targeting the SARS-CoV-2 programmed ribosomal frameshifting RNA from a multiplexed phage display library

Jacob A. Iannuzzelli, Rachel Bonn, Andrew S. Hong, Abhijith Saseendran Anitha, Jermaine L. Jenkins, Joseph E. Wedekind\* and Rudi Fasan\*

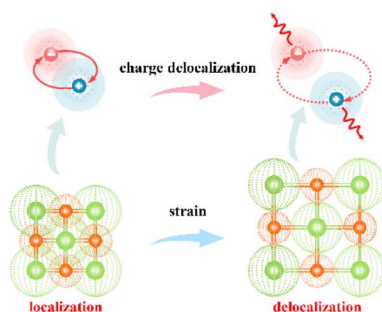
19534



### Regioselectivity switches between anthraquinone precursor fissions involved in bioactive xanthone biosynthesis

Xiao Jing Lv, Chun Zhi Ai, Li Rong Zhang, Xiu Xiu Ma, Juan Juan Zhang, Jia Peng Zhu and Ren Xiang Tan\*

19546



### Strain-induced charge delocalization achieves ultralow exciton binding energy toward efficient photocatalysis

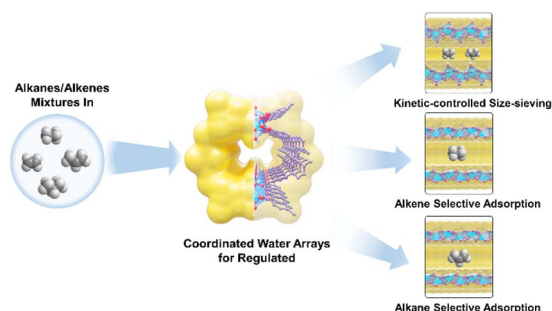
Junyuan Duan, Yinghe Zhao, Yu Wu, Youwen Liu,\* Junnian Chen, Ruouo Yang, Jiazhao Huang, Chuanqi Luo, Mao Wu, Xiaodong Zheng, Pengyu Li, Xueliang Jiang,\* Jianguo Guan\* and Tianyou Zhai



19556

### Three in one: engineering MOF channels via coordinated water arrays for regulated separation of alkanes and alkenes

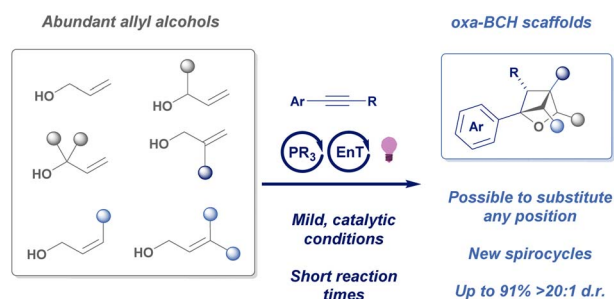
Lu-Lu Ma, Pavel N. Zolotarev, Kang Zhou, Xin Zhou, Jiaqi Liu, Jiafeng Miao, Shenfang Li, Guo-Ping Yang,\* Yao-Yu Wang, Davide M. Proserpio,\* Jing Li\* and Hao Wang\*



19564

### Merging nucleophilic phosphine catalysis and photocatalysis for the rapid assembly of 2-oxabicyclo-[2.1.1]hexane scaffolds from feedstock allyl alcohols

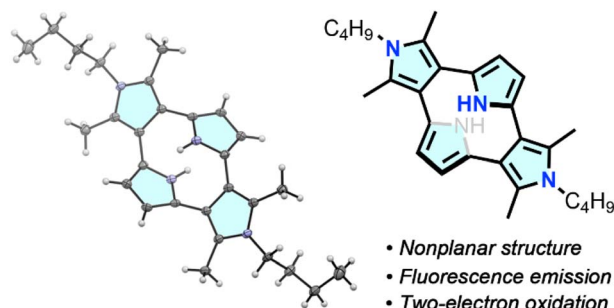
David M. Whalley,\* Luca Carlino, Okky Dwichandra Putra, Niall A. Anderson, Susannah C. Coote and Olivier Lorthioir\*



19571

### Cyclo[4]pyrrole with $\alpha$ - $\beta$ direct linkages

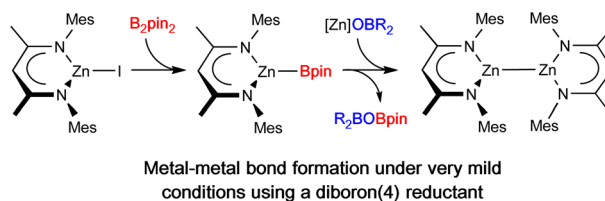
Yuhua Sun, Riku Kitahara, Tomoya Ichino, Yuki Ide, Hisanori Senboku, Soji Shimizu, Takayuki Tanaka\* and Yasuhide Inokuma\*



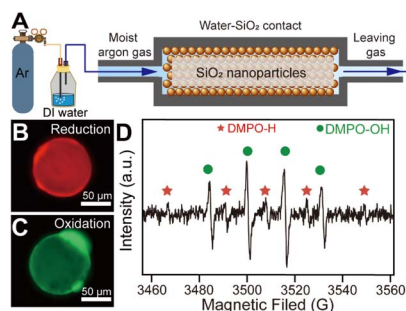
19577

### Zinc borylation and reduction by a diborane(4) species via B-O bond formation

Liam P. Griffin and Simon Aldridge\*



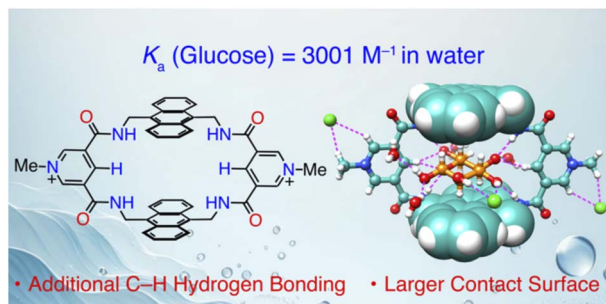
19583



### Simultaneous generation of hydroxyl and hydrogen radicals from $H^+/OH^-$ pairs caused by water–solid contact electrification

Fengjie Chen, Jingde Wu, Dou Wang, Yu Xia, Qingyuan Song, Ying Liang, Pu Wang, Bolei Chen,<sup>\*</sup> Yong Liang, Yongguang Yin, Yawei Wang, Maoyong Song and Guibin Jiang

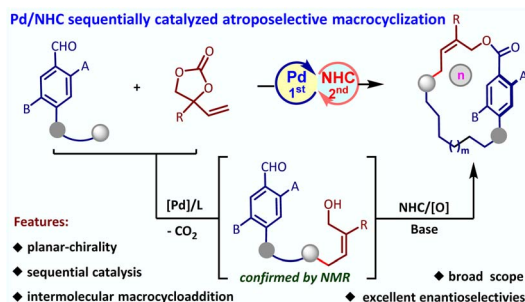
19588



### From small changes to big gains: pyridinium-based tetralactam macrocycle for enhanced sugar recognition in water

Canjia Zhai, Ethan Cross Zulueta, Alexander Mariscal, Chengkai Xu, Yunpeng Cui, Xudong Wang, Huang Wu, Carson Doan, Lukasz Wojtas, Haixin Zhang, Jianfeng Cai, Libin Ye, Kun Wang and Wenqi Liu<sup>\*</sup>

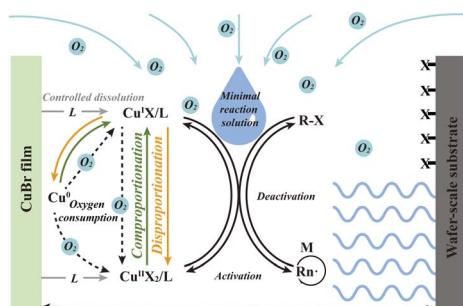
19599



### Pd/NHC sequentially catalyzed atroposelective synthesis of planar-chiral macrocycles

Gongming Yang, Shangde Liu, Shujie Ji, Xingsen Wu and Jian Wang<sup>\*</sup>

19604



### CuBr-mediated surface-initiated controlled radical polymerization in air

Menglu Chen, Shuai You, Tingting Guo, Haohao Ren, Longzu Zhu, Peize Wang, Wenbo Sheng,<sup>\*</sup> Chenliang Gong<sup>\*</sup> and Wei Li<sup>\*</sup>

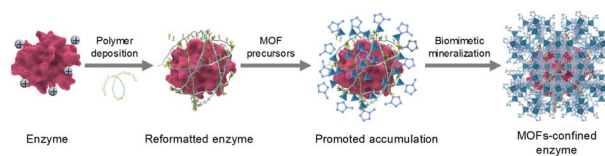


## EDGE ARTICLES

19609

### A polymer deposition-mediated surface-charge reformation strategy: reversing the MOF biomineralization behavior

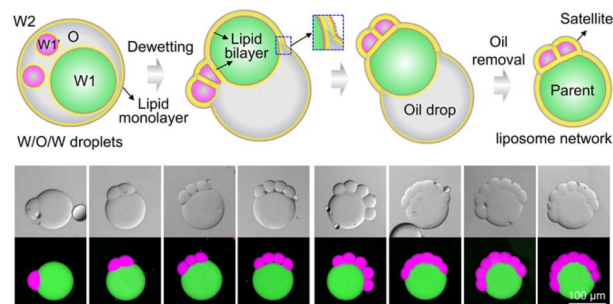
Yanbin Xu, Huangsheng Yang, Anlian Huang, Linjing Tong, Wei Huang, Guosheng Chen,\* Wei Yi,\* Siming Huang\* and Gangfeng Ouyang



19619

### Dynamic satellite–parent liposome networks for quantitative microreactions

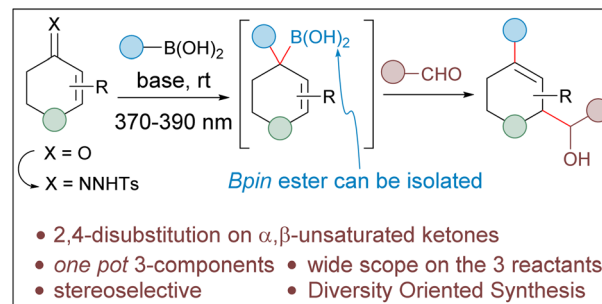
Jia-Qi Tian and Nan-Nan Deng\*



19626

### Photochemical carboborylation and three-component difunctionalization of $\alpha,\beta$ -unsaturated ketones with boronic acids via tosylhydrazones

Álvaro Valdés-Maqueda, Manuel Plaza\* and Carlos Valdés\*



## CORRECTION

19634

### Correction: A new computational methodology for the characterization of complex molecular environments using IR spectroscopy: bridging the gap between experiments and computations

Laura X. Sepulveda-Montaño, Johan F. Galindo and Daniel G. Kuroda\*

