

# Chemical Science

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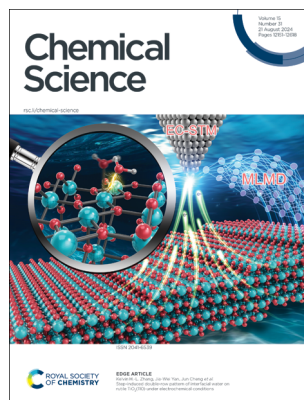
## IN THIS ISSUE

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### Cover

See Tomohiro Seki *et al.*, pp. 12258–12263. Image reproduced by permission of Tomohiro Seki from *Chem. Sci.*, 2024, 15, 12258.



### Inside cover

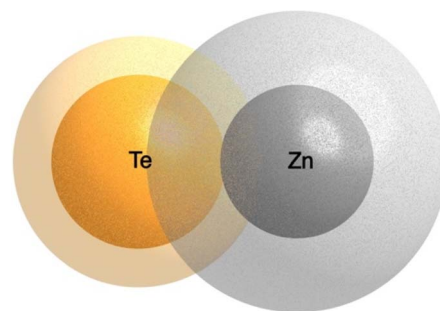
See Kelvin H.-L. Zhang, Jia-Wei Yan, Jun Cheng *et al.*, pp. 12264–12269. Image reproduced by permission of Jun Cheng from *Chem. Sci.*, 2024, 15, 12264.

## COMMENTARY

12166

### A further focus on penetration indices of misfit van der Waals crystals

Jorge Echeverría and Santiago Alvarez

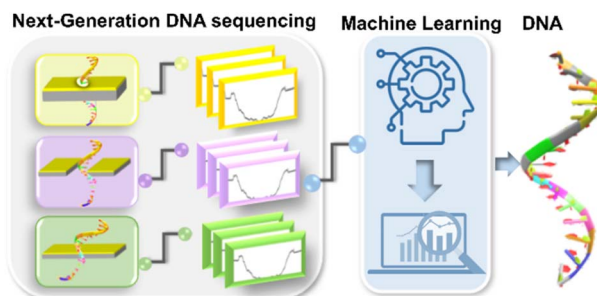


## PERSPECTIVE

12169

### Machine learning empowered next generation DNA sequencing: perspective and prospectus

Sneha Mittal, Milan Kumar Jena and Biswarup Pathak\*



# Environmental Science: Atmospheres

 GOLD  
OPEN  
ACCESS

Connecting communities  
and inspiring new ideas

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Fundamental questions  
Elemental answers



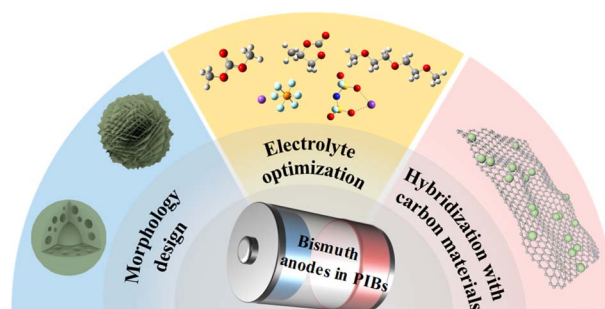


## REVIEWS

12189

**Strategies to boost the electrochemical performance of bismuth anodes for potassium-ion batteries**

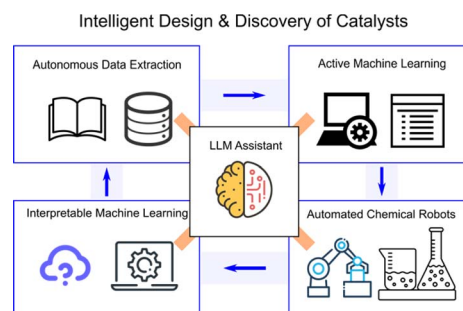
Xunzhu Zhou, Xiaomin Chen, Wenxi Kuang, Xiaosa Zhang, Xingqiao Wu, Xiang Chen, Chaofeng Zhang,\* Lin Li\* and Shu-Lei Chou\*



12200

**Automation and machine learning augmented by large language models in a catalysis study**

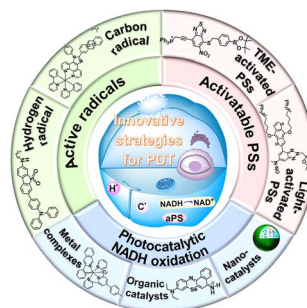
Yuming Su, Xue Wang, Yuanxiang Ye, Yibo Xie, Yujing Xu, Yibin Jiang\* and Cheng Wang\*



12234

**Recent advances for enhanced photodynamic therapy: from new mechanisms to innovative strategies**

Xia Wang, Jinlei Peng, Chi Meng and Fude Feng\*

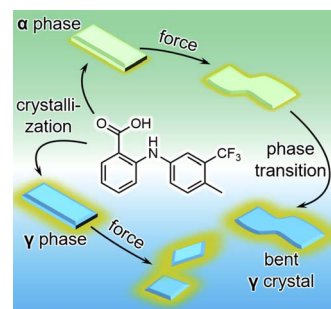


## EDGE ARTICLES

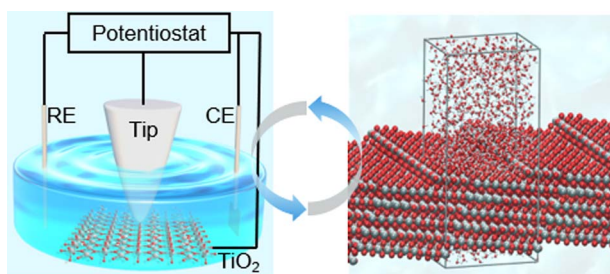
12258

**Preparation of intrinsically fragile bent crystals**

Tomohiro Seki,\* Shiori Kobayashi, Rintaro Ishikawa, Keigo Yano, Takumi Matsuo and Shotaro Hayashi



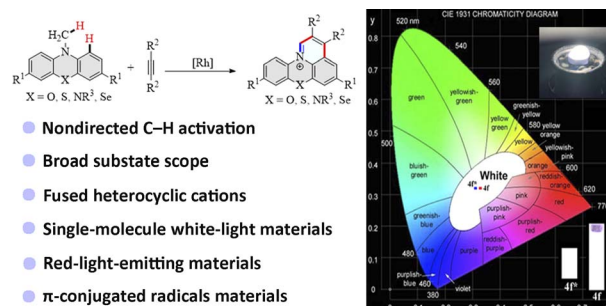
12264



### Step-induced double-row pattern of interfacial water on rutile TiO<sub>2</sub>(110) under electrochemical conditions

Yan Sun, Cheng-Rong Wu, Feng Wang, Rui-Hao Bi, Yong-Bin Zhuang, Shuai Liu, Ming-Shu Chen, Kelvin H.-L. Zhang,\* Jia-Wei Yan,\* Bing-Wei Mao, Zhong-Qun Tian and Jun Cheng\*

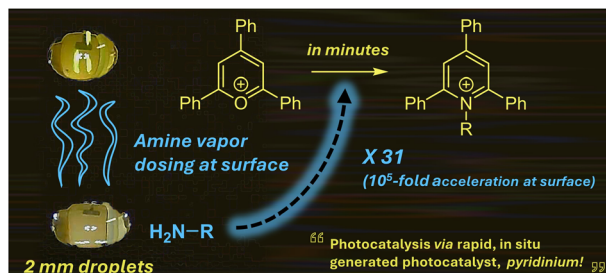
12270



### Rh(III)-catalyzed building up of used heterocyclic cations: facile access to white-light-emitting materials

Jingxian Zhang, Tao Sun, Kangmin Wang, Ruike Hu, Chunlin Zhou, Haibo Ge\* and Bijin Li\*

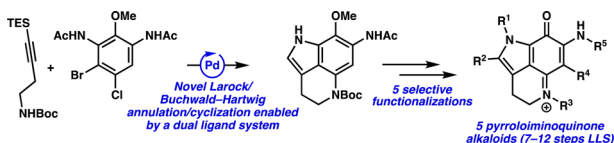
12277



### Reaction acceleration at the surface of a levitated droplet by vapor dosing from a partner droplet

Lingqi Qiu, Xilai Li, Dylan T. Holden and R. Graham Cooks\*

12284



### Divergent total syntheses of pyrroloiminoquinone alkaloids enabled by the development of a Larock/Buchwald-Hartwig annulation/cyclization

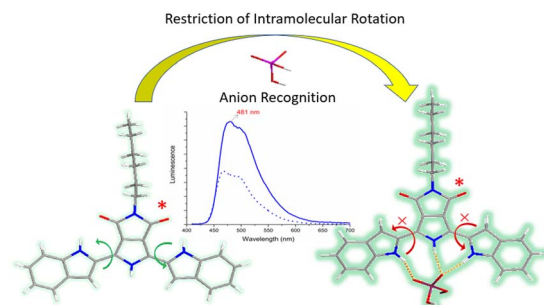
Samir P. Rezgui, Jonathan Farhi, Hao Yu, Zachary P. Sercel, Scott C. Virgil and Brian M. Stoltz\*



12291

## Intensified electrochemiluminescence and photoluminescence *via* supramolecular anion recognition interactions

Jun Cheng, Liuqing Yang, Ruiyao Wang, James A. Wisner, Zhifeng Ding\* and Hong-Bo Wang\*

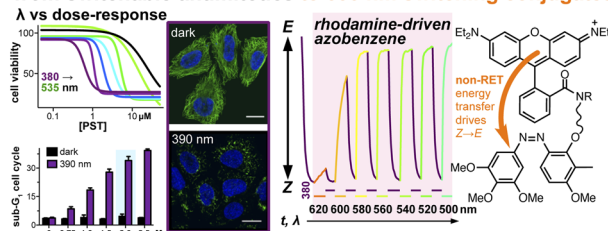


12301

## A photo-SAR study of photoswitchable azobenzene tubulin-inhibiting antimitotics identifying a general method for near-quantitative photocontrol

Martin Reynders, Matgorzata Garścia, Adrian Müller-Deku, Maximilian Wranik, Kristina Krauskopf, Luis de la Osa de la Rosa, Konstantin Schaffer, Anna Jötten, Alexander Rode, Valentin Stierle, Yvonne Kraus, Benedikt Baumgartner, Ahmed Ali, Andrei Bubeneck, Trina Seal, Michel O. Steinmetz, Philipp Paulitschke and Oliver Thorn-Seshold\*

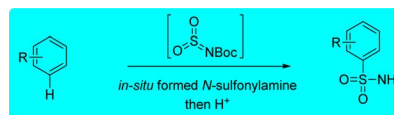
from switchable antimitotics to 600 nm switching conjugates



12310

## Metal-free introduction of primary sulfonamide into electron-rich aromatics

Ming-Ming Wang\* and Kai Johnsson\*

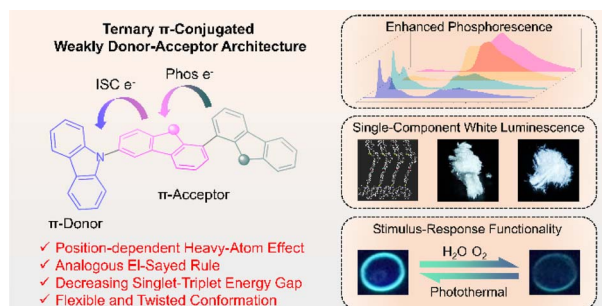


- Metal & catalyst free
- Gram scale synthesis
- Mild reaction conditions
- Late-stage functionalization

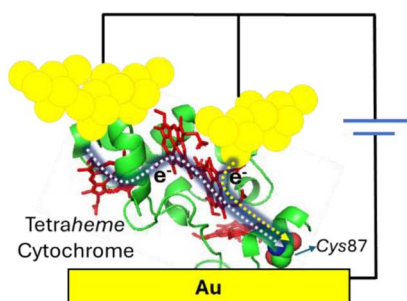
12316

## Utilizing weakly donor–acceptor ternary $\pi$ -conjugated architecture to achieve single-component white luminescence and stimulus-responsive room-temperature phosphorescence

Wenbin Huang, Yuxin Zhu, Xinwei Xie, Guanqun Tang, Kang Zhou, Lijuan Song\* and Zikai He\*



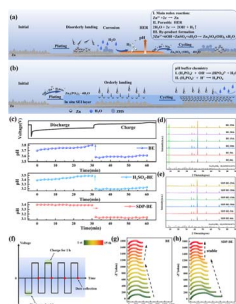
12326



### Shallow conductance decay along the heme array of a single tetraheme protein wire

Kavita Garg, Zdenek Futera, Xiaojing Wu, Yongchan Jeong, Rachel Chiu, Varun Chittari Pisharam, Tracy Q. Ha, Albert C. Aragonès, Jessica H. van Wonderen, Julea N. Butt,\* Jochen Blumberger\* and Ismael Díez-Pérez\*

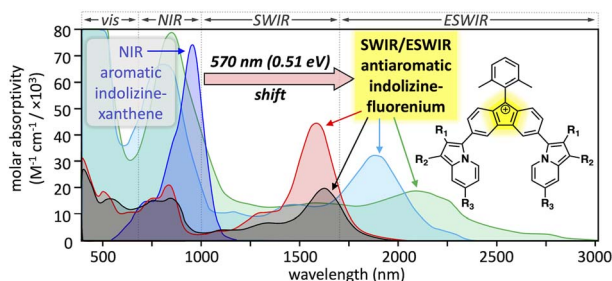
12336



### Dual-function additive enables a self-regulatory mechanism to balance cathode–anode interface demands in Zn||MnO<sub>2</sub> batteries

Yuying Han, Fangzheng Wang, Lijin Yan, Liang Luo, Yuan Qin, Chong Zhu, Jiangyu Hao, Qizhi Chen,\* Xuefeng Zou,\* Yang Zhou\* and Bin Xiang\*

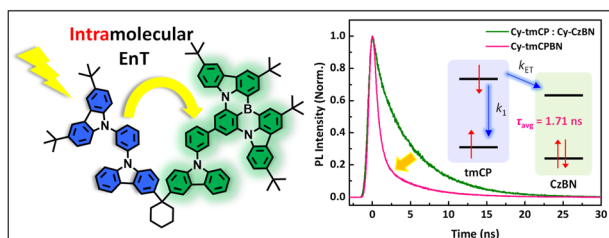
12349



### Extended shortwave infrared absorbing antiaromatic fluorenium-indolizine chromophores

William E. Meador, Matthew A. Saucier, Max R. Tucker, Nicholas A. Kruse, Alexander J. Mobley, Connor R. Brower, Sean R. Parkin, Kensha M. Clark, Nathan I. Hammer, Gregory S. Tschumper and Jared H. Delcamp\*

12361



### Effect of intramolecular energy transfer in a dual-functional molecular dyad on the performance of solution-processed TADF OLEDs

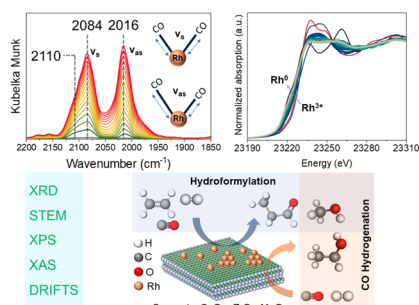
Na Yeon Kwon, Haeun Kwak, Ha Yeon Kim, Su Hong Park, Jin Young Park, Min Ji Kang, Chang Woo Koh, Sungham Park,\* Min Ju Cho\* and Dong Hoon Choi\*



12369

## Understanding the role of supported Rh atoms and clusters during hydroformylation and CO hydrogenation reactions with *in situ/operando* XAS and DRIFT spectroscopy

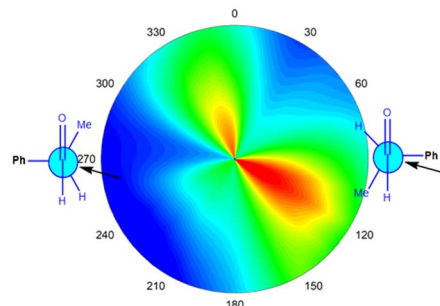
Bidyut Bikash Sarma,\* Dominik Neukum, Dmitry E. Doronkin, Ajai Raj Lakshmi Nilayam, Lorena Baumgarten, Bärbel Krause and Jan-Dierk Grunwaldt



12380

## Origin of the Felkin–Anh(–Eisenstein) model: a quantitative rationalization of a seminal concept

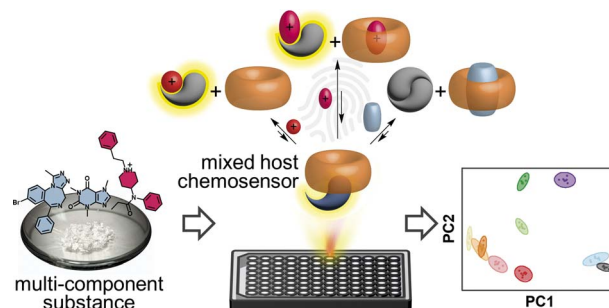
Daniel González-Pinardo, F. Matthias Bickelhaupt and Israel Fernández\*



12388

## Mixed host co-assembled systems for broad-scope analyte sensing

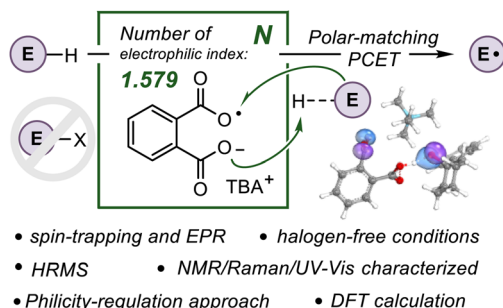
Allison J. Selinger, Joana Krämer, Eric Poarch, Dennis Hore, Frank Biedermann\* and Fraser Hof\*



12398

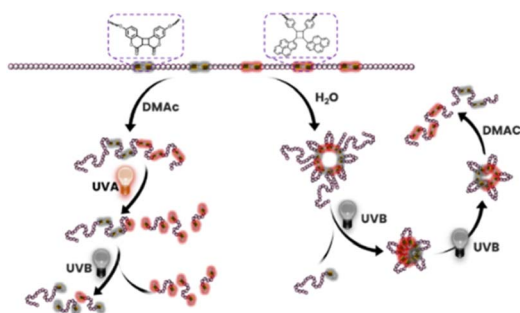
## Revealing the nature of covalently tethered distonic radical anions in the generation of heteroatom-centered radicals: evidence for the polarity-matching PCET pathway

Kang Fu, Xihui Yang, Zhiyou Yu, Lijuan Song\* and Lei Shi\*





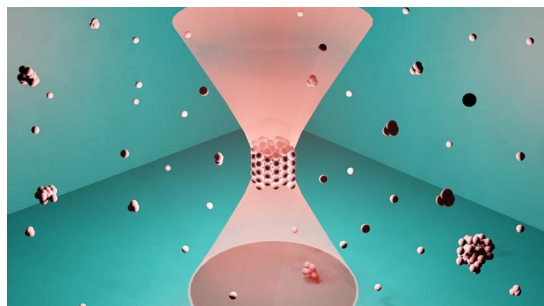
12410



### Main chain selective polymer degradation: controlled by the wavelength and assembly

Phuong T. Do, Federica Sbordone, Henrik Kalmer, Anna Sokolova, Chao Zhang, Linh Duy Thai, Dmitri V. Golberg, Robert Chapman, Berwyck L. J. Poad\* and Hendrik Frisch\*

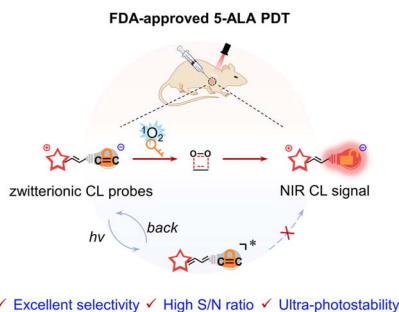
12420



### Amorphous aggregates with a very wide size distribution play a central role in crystal nucleation

Zhiyu Liao, Ankita Das, Christina Glen Robb, Rebecca Beveridge and Klaas Wynne\*

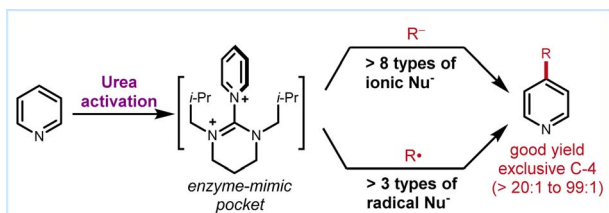
12431



### A *de novo* zwitterionic strategy of ultra-stable chemiluminescent probes: highly selective sensing of singlet oxygen in FDA-approved phototherapy

Yao Lu, Yutao Zhang, Xia Wu, Ruihua Pu, Chenxu Yan, Weimin Liu, Xiaogang Liu, Zhiqian Guo\* and Wei-Hong Zhu

12442



### Unified ionic and radical C-4 alkylation and arylation of pyridines

Qiu Shi, Xiaofeng Huang, Ruizhi Yang and Wenbo H. Liu\*

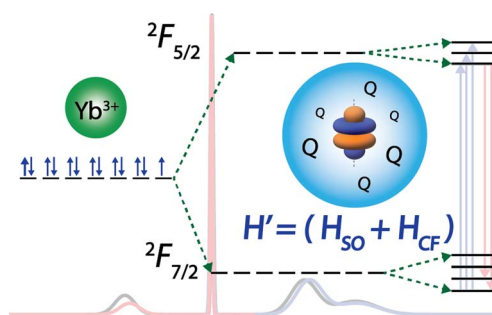




12451

### Elucidating ultranarrow $^2F_{7/2}$ to $^2F_{5/2}$ absorption in ytterbium(III) complexes

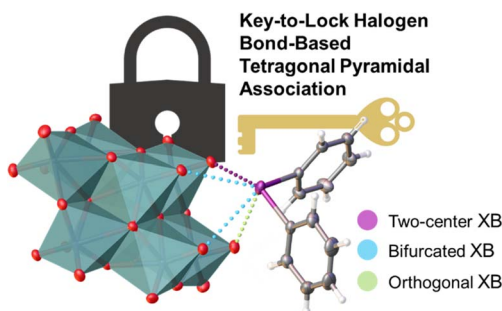
Barry Y. Li, Claire E. Dickerson, Ashley J. Shin, Changling Zhao, Yi Shen, Yongjia He, Paula L. Diaconescu, Anastassia N. Alexandrova and Justin R. Caram\*



12459

### Key-to-lock halogen bond-based tetragonal pyramidal association of iodonium cations with the lacune rims of beta-octamolybdate

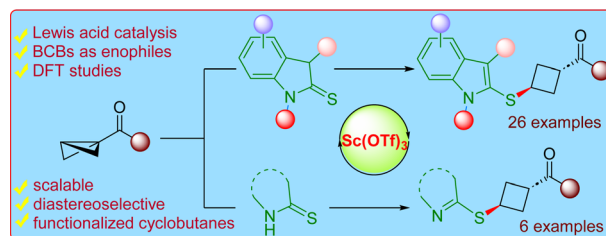
Natalia S. Soldatova, Amirbek D. Radzhabov, Daniil M. Ivanov, Sergi Burguera, Antonio Frontera, Pavel A. Abramov,\* Pavel S. Postnikov\* and Vadim Yu. Kukushkin\*



12473

### Lewis acid-catalyzed diastereoselective formal ene reaction of thioindolinones/thiolactams with bicyclobutanes

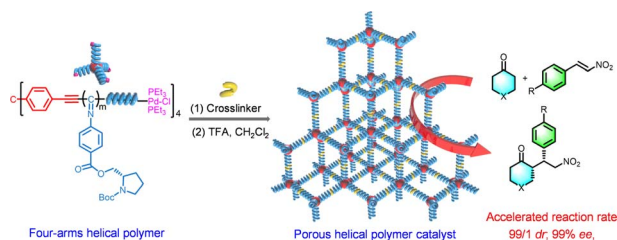
Avishek Guin,\* Shiksha Deswal, Mahesh Singh Harariya and Akkattu T. Biju\*



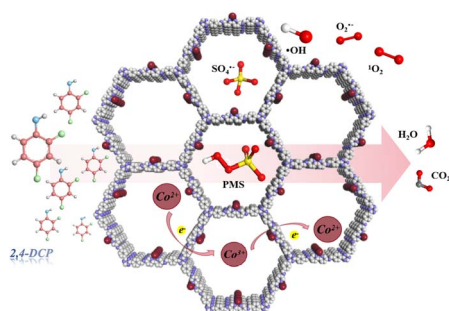
12480

### Helical polyisocyanide-based macroporous organic catalysts for asymmetric Michael addition with high efficiency and stereoselectivity

Xun-Hui Xu, Run-Tan Gao, Shi-Yi Li, Li Zhou,\* Na Liu and Zong-Quan Wu\*



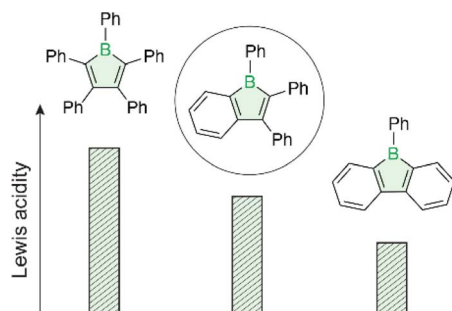
12488



### A cobalt-modified covalent organic framework enables highly efficient degradation of 2,4-dichlorophenol in high concentrations through peroxymonosulfate activation

Yunchao Ma, Yuhang Han, Yuxin Yao, Tianyu Zhou, Dongshu Sun, Chunbo Liu,\* Guangbo Che,\* Bo Hu,\* Valentin Valtchev and Qianrong Fang

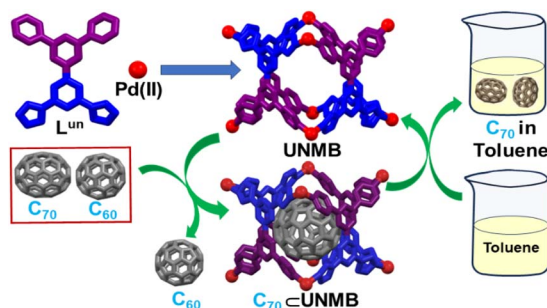
12496



### The forgotten borole: synthesis, properties and reactivity of a 1-boraindene

Nele Wieprecht, Ivo Krummenacher, Leonie Wüst, Maximilian Michel, Sonja Fuchs, Samuel Nees, Marcel Härterich and Holger Braunschweig\*

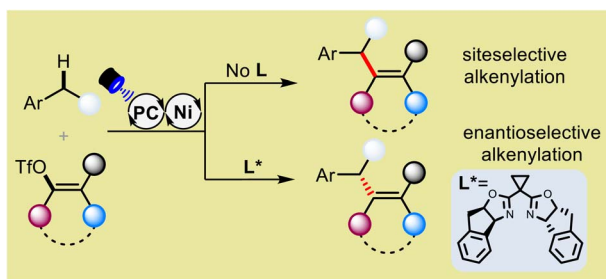
12502



### Formation of a low-symmetry Pd<sub>8</sub> molecular barrel employing a hetero donor tetradentate ligand, and its use in the binding and extraction of C<sub>70</sub>

Dharmraj Prajapati, Jack K. Clegg and Partha Sarathi Mukherjee\*

12511



### Stereoselective benzylic C(sp<sup>3</sup>)-H alkenylation enabled by metallaphotoredox catalysis

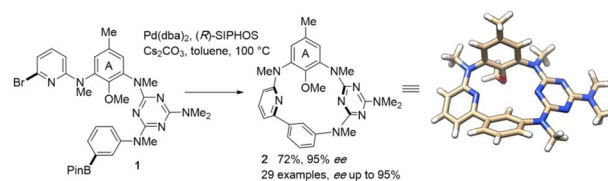
Yantao Li, Haonan Bai, Qi Gao, Kai Liu, Jie Han, Weipeng Li, Chengjian Zhu\* and Jin Xie\*



12517

## Inherently chiral nor-heteracalixarenes: design and synthesis *via* enantioselective intramolecular Suzuki–Miyaura reaction

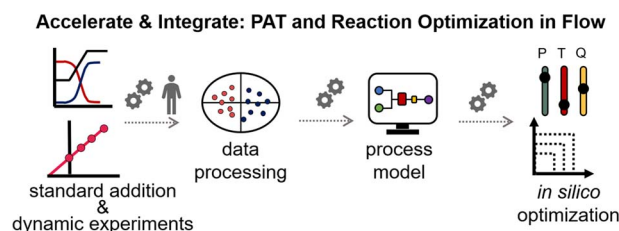
Yi-Fan Jiang, Shuo Tong,<sup>\*</sup> Jieping Zhu and Mei-Xiang Wang



12523

## Simultaneous reaction- and analytical model building using dynamic flow experiments to accelerate process development

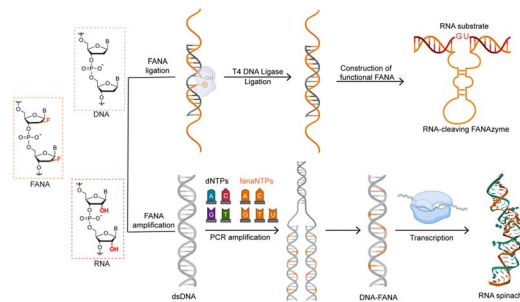
Peter Sagmeister, Lukas Melnizky, Jason D. Williams<sup>\*</sup> and C. Oliver Kappe<sup>\*</sup>



12534

## Advancing the enzymatic toolkit for 2'-fluoro arabinonucleic acid (FANA) manipulation: phosphorylation, ligation, replication, and templating RNA transcription

Yingyu Liu, Jun Wang, Yashu Wu and Yajun Wang<sup>\*</sup>



12543

## Development of non-closed silver clusters by transition-metal-coordination-cluster substituted polyoxometalate templates

Rui Ge, Ping-Wei Cai, Cai Sun, Yan-Qiong Sun, Xin-Xiong Li<sup>\*</sup> and Shou-Tian Zheng<sup>\*</sup>





**21 HCN Supported Noble-metal-based alloys**

**Cation exchange & Spatial confinement**

**1. Generality**

**2. Durability**


**Durable methanol oxidation in acidic medium**

**This work**

Guanzhen Chen, Jie Zhang, Wen Chen, Ruihu Lu,  
Chao Ma, Ziyun Wang\* and Yunhu Han\*

Yingcui Bu, Zhi-Peng Yu, Zhou Lu, Haoran Wang,  
Yu Deng, Xiaojiao Zhu\* and Hongping Zhou\*

### Electron Transfer Mechanism



The diagram illustrates the electron transfer mechanism in photosynthesis. It shows a central protein complex (PSII) with yellow wavy lines representing the light-harvesting complex. A red lightning bolt labeled  $d-S_T$  indicates the absorption of light energy. On the left, a cycle shows the oxidation of NADPH to  $NADP^+$ , releasing an electron ( $e^-$ ). On the right, a cycle shows the reduction of  $H_2O$  to  $H\cdot$ , which also releases an electron ( $e^-$ ). The electrons from these cycles are transferred to the protein complex.

Photoregulation of molecular conformation rather than molecular structure

UV ON  
UV OFF

Conformation Change

Assembly Transformation

Order-to-Order Phase Transition

Persistent room-temperature photophorescence characteristic with water resistance

Mouwei Liu, Bin Wu, Glib V. Baryshnikov, Shen Shen,  
Hao Sun, Xinyan Gu, Hans Ågren, Yifei Xu, Qi Zou,\*  
Da-Hui Qu and Liangliang Zhu\*

High catalytic activity  
High catalytic stability  
High faradaic efficiency

$H_2$   
 $H_2O$

$V_0$ -rich CuO/CF

Xu Yang, Enhui Wei, Yuan Dong, Yu Fan, Hongtao Gao,  
Xiliang Luo\* and Wenlong Yang\*

12589

## Heptacyclic aromatic hydrocarbon isomers with two azulene units fused

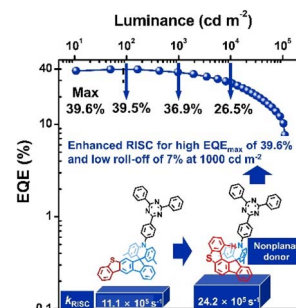
Jianwen Guo, Fangxin Du, Bo Yu, Pengcheng Du, Haoyuan Li, Jianhua Zhang and Hanshen Xin\*



12598

## Nonplanar structure accelerates reverse intersystem crossing of TADF emitters: nearly 40% EQE and relieved efficiency roll off

He Liu, Yang Liu, Guohao Chen, Yuan Meng, Hao Peng, Jingsheng Miao and Chuluo Yang\*



12606

## Achieving efficient and stable blue thermally activated delayed fluorescence organic light-emitting diodes based on four-coordinate fluoroboron emitters by simple substitution molecular engineering

Panpan Li, Shiu-Lun Lai, Ziyong Chen, Wai Kit Tang, Ming-Yi Leung, Maggie Ng, Wing-Kei Kwok, Mei-Yee Chan\* and Vivian Wing-Wah Yam\*

### Blue Four-Coordinate Boron TADF Emitters

