

## IN THIS ISSUE

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### Cover

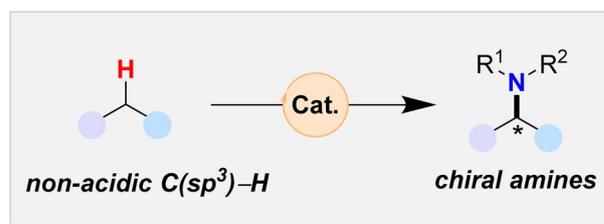
See Oleg V. Larionov *et al.*, pp. 13384–13391. Image reproduced by permission of Oleg V. Larionov from *Chem. Sci.*, 2023, 14, 13384.

## PERSPECTIVES

13278

### Recent developments for intermolecular enantioselective amination of non-acidic C(sp<sup>3</sup>)-H bonds

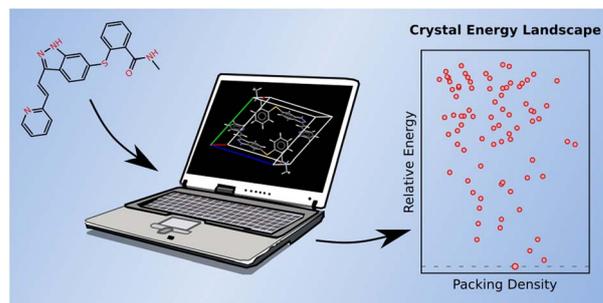
Heng-Hui Li, Xuemeng Chen and Søren Kramer\*



13290

### Frontiers of molecular crystal structure prediction for pharmaceuticals and functional organic materials

Gregory J. O. Beran



# Chemical Science

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## PERSPECTIVES

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## Two-dimensional mesoporous metals: a new era for designing functional electrocatalysts

Hao Lv and Ben Liu\*

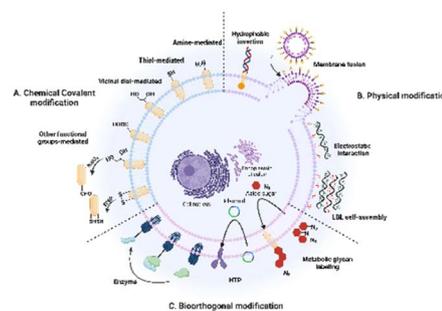


## REVIEWS

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## Advancing cell surface modification in mammalian cells with synthetic molecules

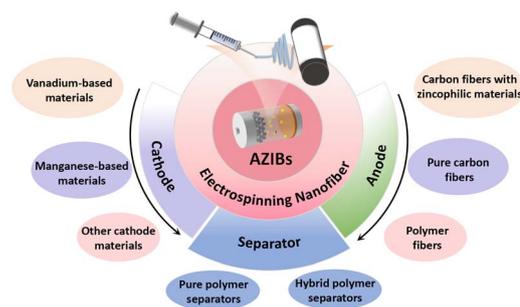
He Yang, Lihua Yao, Yichen Wang, Gaojian Chen\* and Hong Chen\*



13346

## Recent advances in electrospinning nanofiber materials for aqueous zinc ion batteries

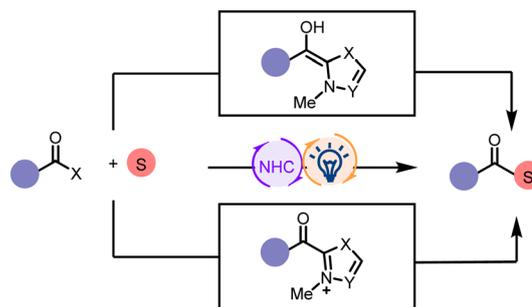
Sinian Yang, Shunshun Zhao and Shimou Chen\*



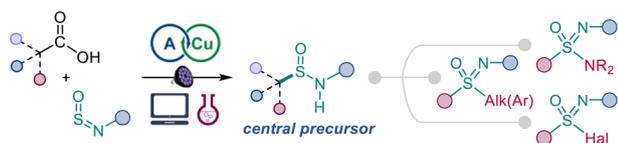
13367

## Recent advances in combining photo- and N-heterocyclic carbene catalysis

Xiaochen Wang, Senhui Wu, Rongxin Yang, Hongjian Song, Yuxiu Liu and Qingmin Wang\*



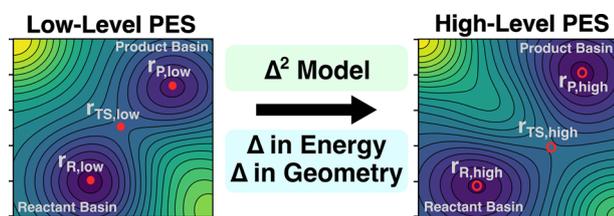
13384



### Kinetically-driven reactivity of sulfinylamines enables direct conversion of carboxylic acids to sulfinamides

Hang T. Dang, Arka Porey, Sachchida Nand, Ramon Trevino, Patrick Manning-Lorino, William B. Hughes, Seth O. Fremin, William T. Thompson, Shree Krishna Dhakal, Hadi D. Arman and Oleg V. Larionov\*

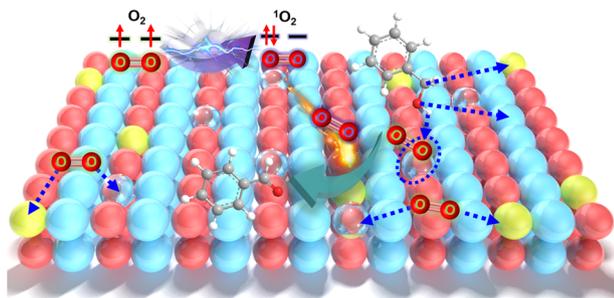
13392



### $\Delta^2$ machine learning for reaction property prediction

Qiyuan Zhao, Dylan M. Anstine, Olexandr Isayev\* and Brett M. Savoie\*

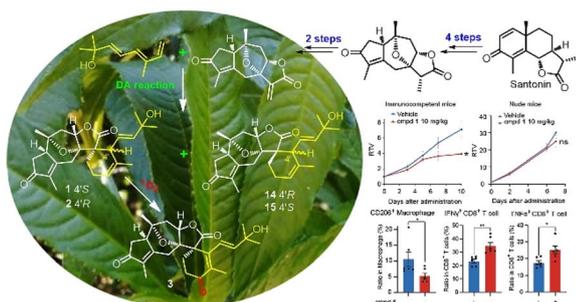
13402



### Spontaneous generation of singlet oxygen on microemulsion-derived manganese oxides with rich oxygen vacancies for efficient aerobic oxidation

Jun Tang, Junbao Chen, Zhanyu Zhang, Qincheng Ma, Xiaolong Hu, Peng Li, Zhiqiang Liu, Peixin Cui, Chao Wan,\* Qingping Ke,\* Lei Fu, Jeonghun Kim, Takashi Hamada, Yunqing Kang\* and Yusuke Yamauchi\*

13410



### Unprecedented sesterterpenoids, orientanoids A–C: discovery, bioinspired total synthesis and antitumor immunity

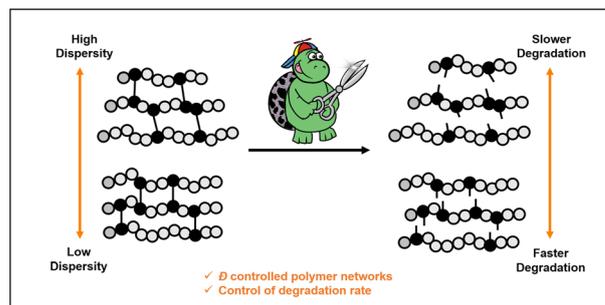
Cheng-Yu Zheng, Jin-Xin Zhao, Chang-Hao Yuan, Xia Peng, Meiyu Geng, Jing Ai,\* Yao-Yue Fan\* and Jian-Min Yue\*



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### Controlling primary chain dispersity in network polymers: elucidating the effect of dispersity on degradation

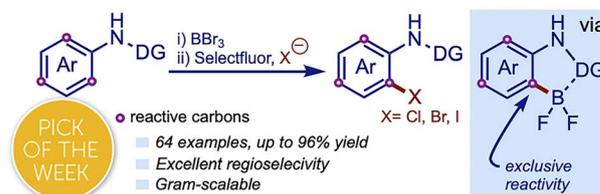
Takanori Shimizu, Richard Whitfield,\* Glen R. Jones, Ibrahim O. Raji, Dominik Konkolewicz, Nghia P. Truong and Athina Anastasaki\*



13429

### Regioselective *ortho* halogenation of *N*-aryl amides and ureas *via* oxidative halodeboronation: harnessing boron reactivity for efficient C–halogen bond installation

Ganesh H. Shinde, Ganesh S. Ghotekar, Francoise M. Amombo Noa, Lars Öhrström, Per-Ola Norrby and Henrik Sundén\*

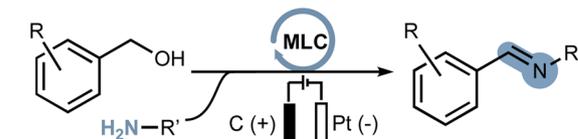


13437

### Merging electrocatalytic alcohol oxidation with C–N bond formation by electrifying metal–ligand cooperative catalysts

Sitthichok Kasemthaveechok, Patrice Gérardo and Niklas von Wolff\*

First molecular electrocatalytic C–N bond formation from alcohols



No amine oxidation  
low reaction potential  
high TON > 60  
> 30 examples

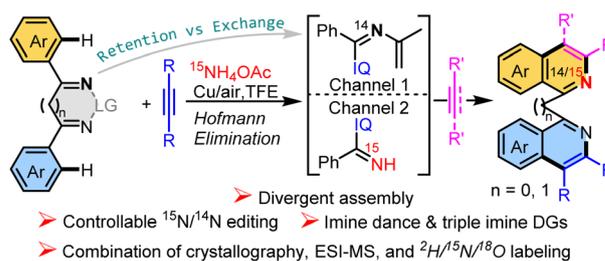
Electrification of MLC-catalysts



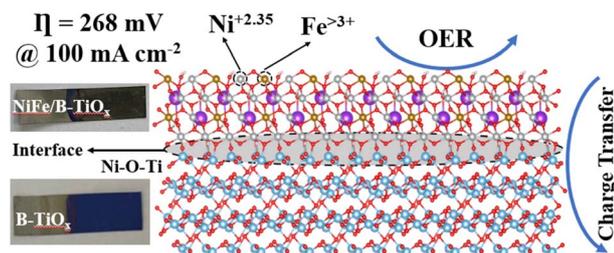
13446

### Mechanistic insights into an $\text{NH}_4\text{OAc}$ -promoted imine dance in Rh-catalysed multicomponent double C–H annulations through an N-retention/exchange dual channel

Shiqing Li,\* Shihai Lv, Yanyan Yang, Peiyan Zhu, Dongbing Zhao\* and Ming-Hua Zeng\*



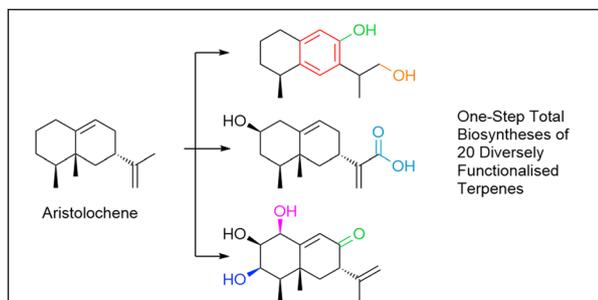
13453



### Defective blue titanium oxide induces high valence of NiFe-(oxy)hydroxides over heterogeneous interfaces towards high OER catalytic activity

Tingxi Zhou, Yifei Yang, Yike Jing, Yuling Hu, Fei Yang, Wei Sun\* and LeiLei He\*

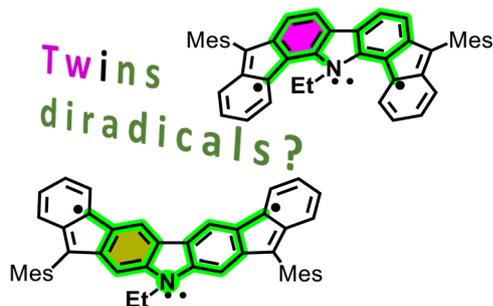
13463



### Rapid discovery of terpene tailoring enzymes for total biosynthesis

Yunlong Sun, Jennifer Gerke, Kevin Becker, Eric Kuhnert, Bart Verwaaijen, Daniel Wibberg, Jörn Kalinowski, Marc Stadler and Russell J. Cox\*

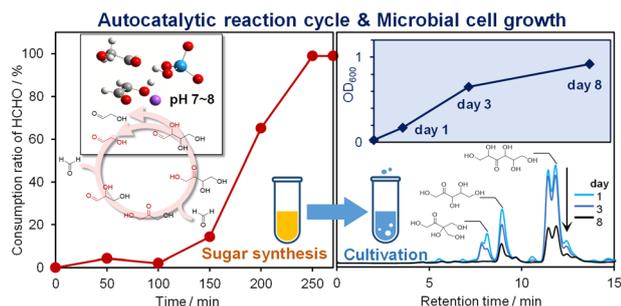
13468



### Isomerism tunes the diradical character of difluorenylpyrroles at constant Hückel-level anti-aromaticity

Ryotaro Moriyasu, Sergio Moles Quintero, Carlos J. Gómez-García, Kazumasa Suzuki, Chitoshi Kitamura, Michihisa Murata, Mercedes Alonso, Juan Casado\* and Shin-ichiro Kato\*

13475



### Construction of an autocatalytic reaction cycle in neutral medium for synthesis of life-sustaining sugars

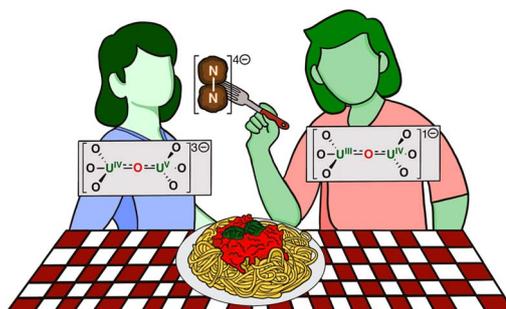
Hiro Tabata, Genta Chikatani, Hiroaki Nishijima, Takashi Harada, Rika Miyake, Souichiro Kato, Kensuke Igarashi, Yoshiharu Mukoyama, Soichi Shirai, Minoru Waki, Yoko Hase\* and Shuji Nakanishi\*



13485

**Dinitrogen cleavage by a dinuclear uranium(III) complex**

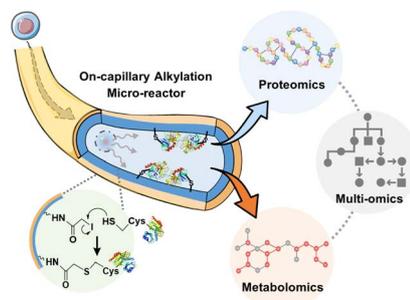
Nadir Jori, Megan Keener, Thayalan Rajeshkumar, Rosario Scopelliti, Laurent Maron\* and Marinella Mazzanti\*



13495

**On-capillary alkylation micro-reactor: a facile strategy for proteo-metabolome profiling in the same single cells**

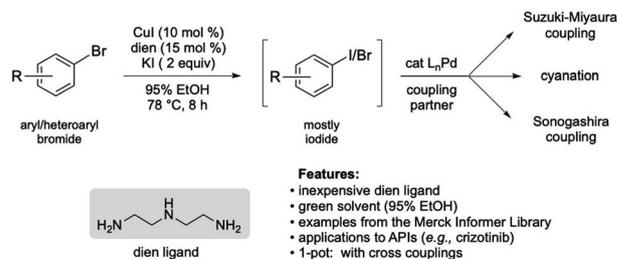
Yingyun He, Huiming Yuan,\* Yu Liang, Xinxin Liu, Xiaozhe Zhang, Yahui Ji, Baofeng Zhao, Kaiguang Yang, Jue Zhang, Shen Zhang, Yukui Zhang and Lihua Zhang\*



13503

**Challenging cross couplings, in water, aided by *in situ* iodination of (hetero)aromatic bromides**

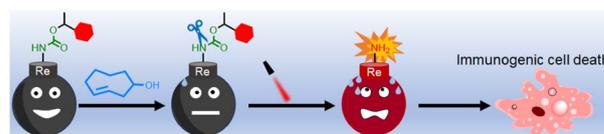
Rohan M. Thomas, David B. Obbard and Bruce H. Lipshutz\*



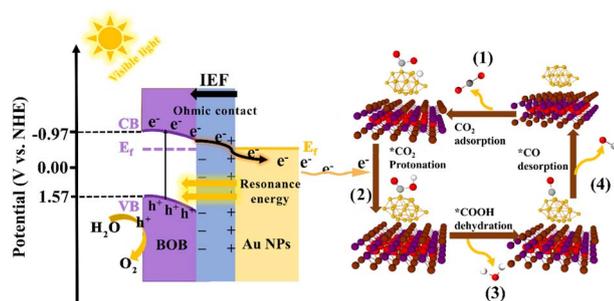
13508

**Bioorthogonal dissociative rhenium(I) photosensitisers for controlled immunogenic cell death induction**

Guang-Xi Xu, Lawrence Cho-Cheung Lee, Peter Kam-Keung Leung, Eunice Chiu-Lam Mak, Justin Shum, Kenneth Yin Zhang, Qiang Zhao and Kenneth Kam-Wing Lo\*



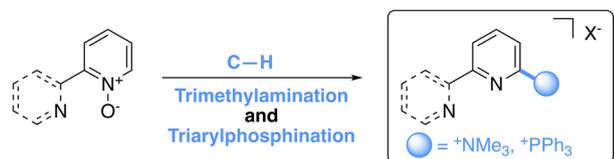
13518



### Synergistic coupling of interface ohmic contact and LSPR effects over Au/Bi<sub>24</sub>O<sub>31</sub>Br<sub>10</sub> nanosheets for visible-light-driven photocatalytic CO<sub>2</sub> reduction to CO

Jie Liu, Yu Xie,\* Yiqiao Wang, Kai Yang, Shuping Su, Yun Ling and Pinghua Chen

13530

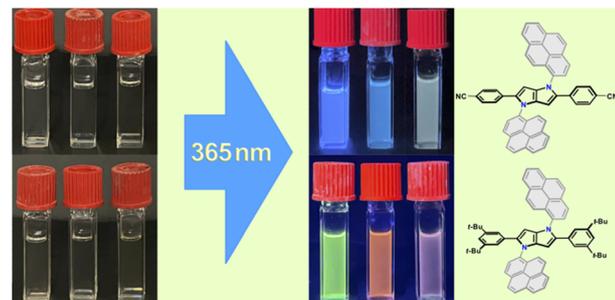


- One Pot
- Modular Synthesis
- Scalable (up to 5 g scale)
- Electrochemistry
- Metal Coordination
- Physical Properties

### Modular preparation of cationic bipyridines and azaarenes via C–H activation

Ryan P. King and Jenny Y. Yang\*

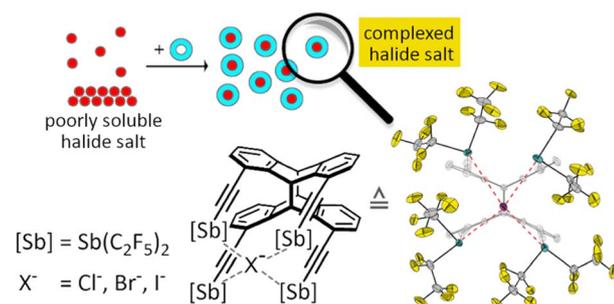
13537



### The magic of biaryl linkers: the electronic coupling through them defines the propensity for excited-state symmetry breaking in quadrupolar acceptor–donor–acceptor fluorophores

John A. Clark, Damian Kusy, Olena Vakuliuk, Maciej Krzeszewski, Krzysztof J. Kochanowski, Beata Koszarna, Omar O'Mari, Denis Jacquemin,\* Daniel T. Gryko\* and Valentine I. Vullev\*

13551



### Poly-pnictogen bonding: trapping halide ions by a tetradentate antimony(III) Lewis acid

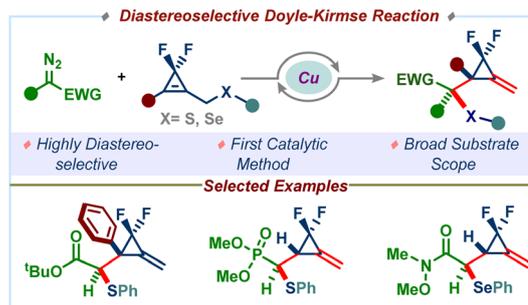
J. Louis Beckmann, Jonas Krieft, Yury V. Vishnevskiy, Beate Neumann, Hans-Georg Stammer and Norbert W. Mitzel\*



13560

### A highly diastereoselective strain-release Doyle–Kirmse reaction: access to functionalized difluoro(methylene)cyclopropanes

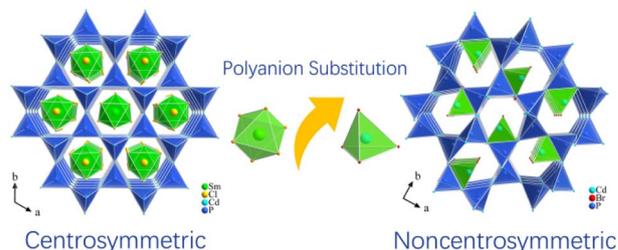
Suparnak Midya and Durga Prasad Hari\*



13568

### The first polyanion-substitution-driven centrosymmetric-to-noncentrosymmetric structural transformation realizing an excellent nonlinear optical supramolecule [Cd<sub>4</sub>P<sub>2</sub>][CdBr<sub>4</sub>]

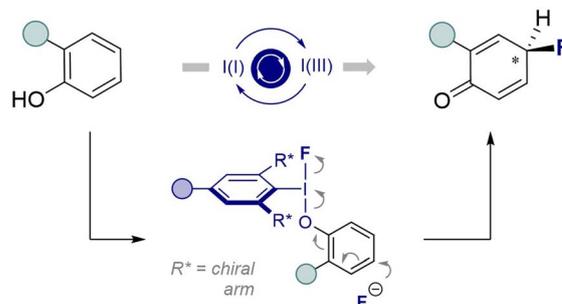
Zhi-Xin Qiu, Zhe-Xiong Zheng, Xiao-Ming Jiang, Bin-Wen Liu\* and Guo-Cong Guo\*



13574

### *para*-Selective dearomatization of phenols by I(I)/I(III) catalysis-based fluorination

Timo Stünkel, Kathrin Siebold, Daichi Okumatsu, Kazuki Murata, Louise Ruyet, Constantin G. Daniliuc and Ryan Gilmour\*



13581

### *Trans*-cyclosulfamidate mannose-configured cyclitol allows isoform-dependent inhibition of GH47 $\alpha$ -D-mannosidases through a bump–hole strategy

Alexandra Males, Ken Kok, Alba Nin-Hill, Nicky de Koster, Sija van den Beukel, Thomas J. M. Beenakker, Gijsbert A. van der Marel, Jeroen D. C. Codée, Johannes M. F. G. Aerts, Herman S. Overkleef, Carme Rovira,\* Gideon J. Davies\* and Marta Artola\*

