

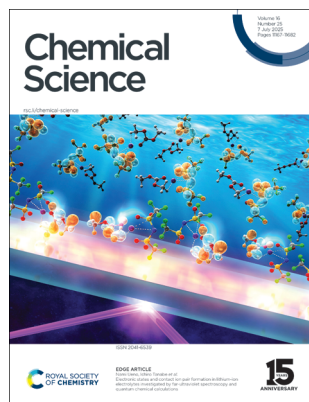
# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(25) 11167–11682 (2025)



**Cover**  
See Nami Ueno, Ichiro Tanabe *et al.*, pp. 11232–11239. Image reproduced by permission of Ichiro Tanabe from *Chem. Sci.*, 2025, **16**, 11232.



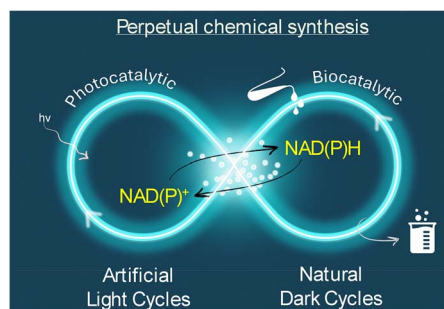
**Inside cover**  
See Kanta Kawai, Tasuku Hirayama *et al.*, pp. 11240–11245. Image reproduced by permission of Kanta Kawai from *Chem. Sci.*, 2025, **16**, 11240.

## PERSPECTIVE

11184

### A path to perpetual chemical synthesis via photocatalytic cofactor regeneration

Vanshika Jain\* and Pramod P. Pillai\*

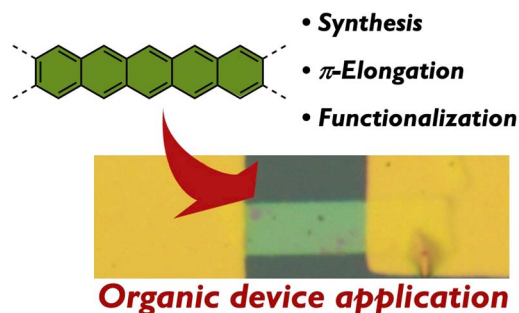


## REVIEW

11204

### Exploring the chemistry of higher acenes: from synthesis to applications

Hironobu Hayashi\* and Hiroko Yamada\*



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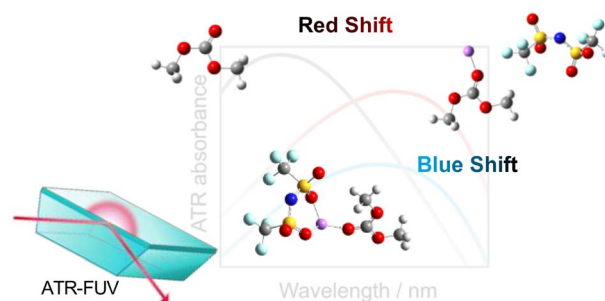
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11232

### Electronic states and contact ion pair formation in lithium-ion electrolytes investigated by far-ultraviolet spectroscopy and quantum chemical calculations

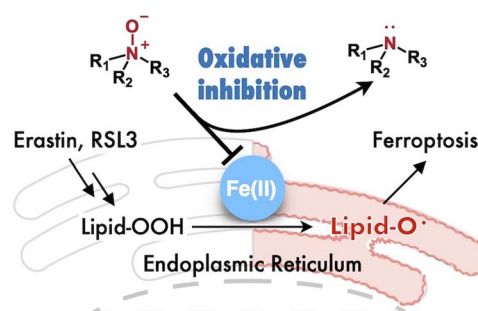
Hitomi Sato, Nami Ueno\* and Ichiro Tanabe\*



11240

### Inhibition of ferroptosis by *N*-oxide-based fluorescent probes *via* selective oxidation of ferrous ions

Kanta Kawai, Rie Haruki, Shunsuke Nozawa, Hideko Nagasawa and Tasuku Hirayama\*



11246

### Preferential survival of prebiotic metallopeptides in the presence of ultraviolet light

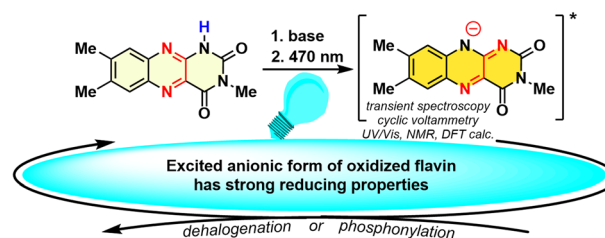
Daniele Rossetto, Serge Nader, Corinna L. Kufner, Gabriella G. Lozano, Linda Cerofolini, Marco Fragai, Vlad Martin-Diaconescu, Barbara Zambelli, Stefano Ciurli, Graziano Guella, Rafat Szabla, Dimitar D. Sasselov and Sheref S. Mansy\*



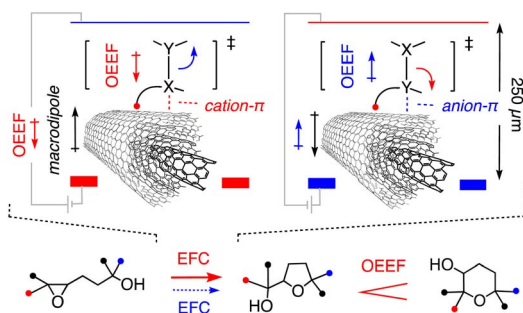
11255

### Introduction of flavin anions into photoredox catalysis: acid–base equilibria of lumichrome allow photoreductions with an anion of an elusive 10-unsubstituted isoalloxazine

Dorota Prukala\*, Ekaterina Zubova, Eva Svobodová, Ludmila Šimková, Naisargi Varma, Josef Chudoba, Jiří Ludvík, Gotard Burdzinski, Iwona Gulaczyk, Marek Sikorski\* and Radek Cibulka\*



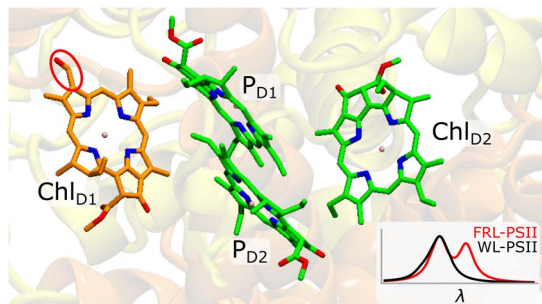
11264



### Response of reaction mechanisms to electric-field catalysis on carbon nanotubes in microfluidic reactors

M. Ángeles Gutiérrez López, Alenka Marsalek, Naomi Sakai and Stefan Matile\*

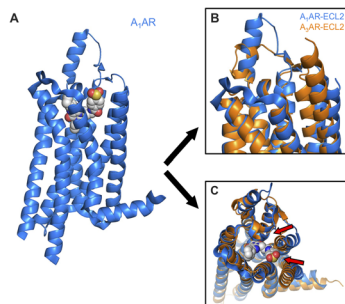
11270



### Modified chlorophyll pigment at Chl<sub>D1</sub> tunes photosystem II beyond the red-light limit

Friederike Allgöwer, Abhishek Sirohiwal, Ana P. Gamiz-Hernandez, Maximilian C. Pöverlein, Andrea Fantuzzi, A. William Rutherford and Ville R. I. Kaila\*

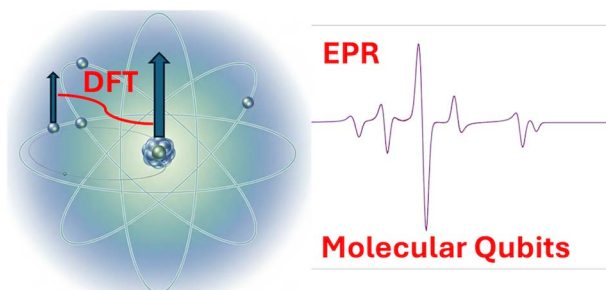
11280



### Enhancing binding affinity predictions through efficient sampling with a re-engineered BAR method: a test on GPCR targets

Minkyu Kim, Jian Jeong, Donghwan Kim, Sangbae Lee\* and Art E. Cho\*

11291



### Exploring hyperfine coupling in molecular qubits

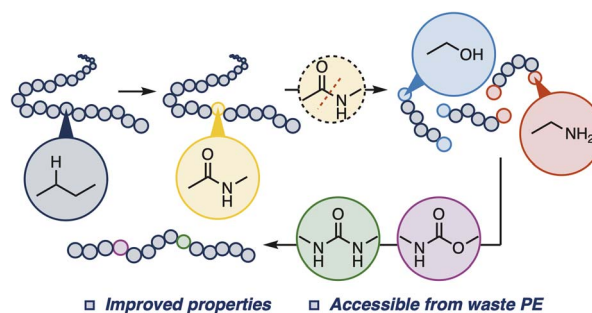
Joan Cardona, Àlex Solé, Pablo Mella, Daniel Aravena,\* Javier Ruiz-Hidalgo,\* Silvia Gómez-Coca\* and Eliseo Ruiz\*



11304

### Backbone editing and deconstruction of polyethylene by Beckmann rearrangement and hydrogenolysis

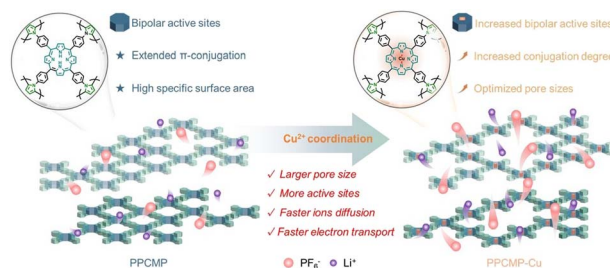
Jake X. Shi, Diane D. Kim, Nicodemo R. Ciccio, Pierre Lahaie-Boivin and John F. Hartwig\*



11311

### Cu-mediated bipolar-type extended $\pi$ -conjugated microporous polymers for lithium-ion battery cathodes with high energy density and fast-charging capability

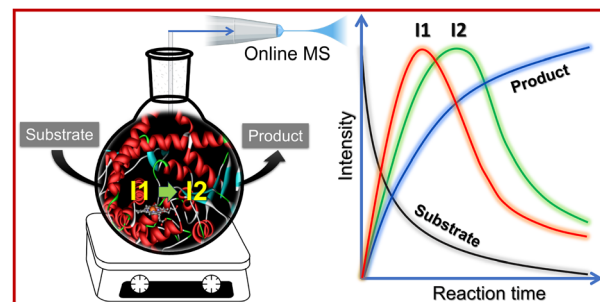
Yitao Li, Ju Duan, Yuzhu Wang, Likuan Teng, He Liu, Jiaqiang Li, Mengqi Liu, Weisi He, Huawei Hu, Lulu Wang, Wei Lyu\* and Yaozu Liao\*



11322

### Real-time capture of reactive intermediates in an enzymatic reaction: insights into a P450-catalyzed oxidation

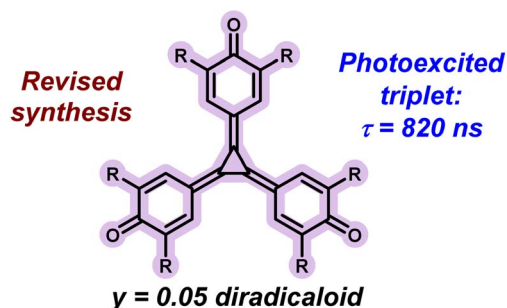
Pragya Pahchan, Abhijit Nandy, Eswarayya Ramireddy\* and Shibdas Banerjee\*



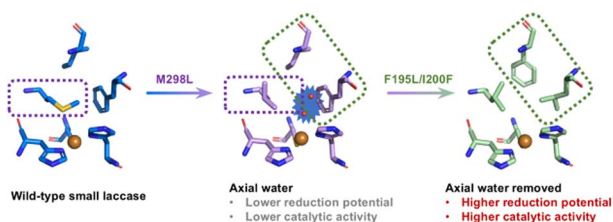
11331

### Photoexcited and ground-state diradical(oid) character in a triquino[3]radialene

Bethany K. Hillier, Damon M. de Clercq, Stephen D. S. Bortolussi, Simona S. Capomolla, Michael P. Nielsen, Katarzyna Młodzikowska-Pienko, Renana Gershoni-Poranne, Timothy W. Schmidt and Martin D. Peeks\*



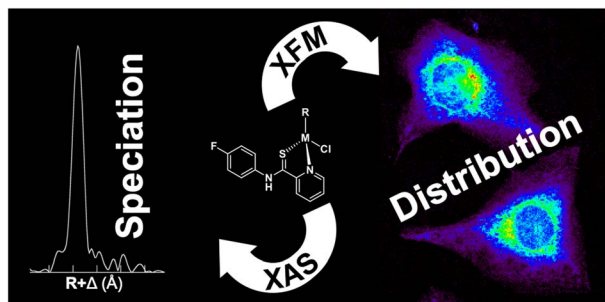
11339



### Unexpected effect of an axial ligand mutation in the type 1 copper center in small laccase: structure-based analyses and engineering to increase reduction potential and activity

Jing-Xiang Wang, Avery C. Vilbert, Lucas H. Williams, Evan N. Mirts, Chang Cui and Yi Lu\*

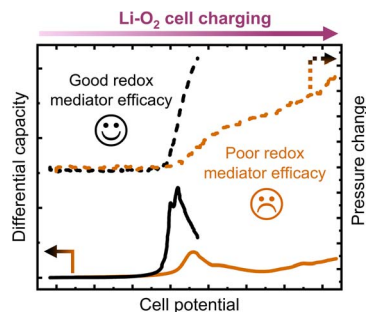
11347



### X-ray fluorescence microscopy and X-ray absorption spectroscopy reveal the stability of the plecstatin-1 scaffold in biological model systems: comparison of Ru, Os and Ir analogues

James H. Lovett, Barry P. Lai, Hugh O. Bloomfield, Ani T. Baker, Matthew P. Sullivan, Christian G. Hartinger and Hugh H. Harris\*

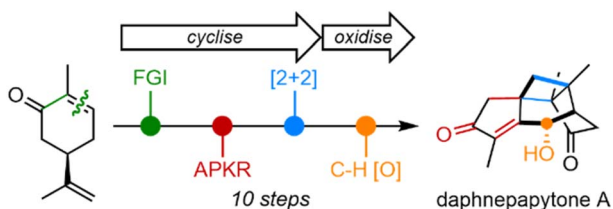
11359



### Multicycle *operando* pressure measurements enable assessment of redox mediator efficacy in lithium-oxygen batteries

Thukshan Samarakoon, Ben Wood, Alex R. Neale, Elliot Coulbeck, Daniel J. Saccomando and Laurence J. Hardwick\*

11375



### Bio-inspired total synthesis of daphnepapytone A

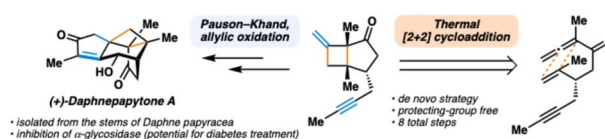
Joan Pereira, Nicolas Casaretto, Gilles Frison and Bastien Nay\*



11381

### Concise total synthesis of the cage-like sesquiterpenoid (+)-daphnepapytone A

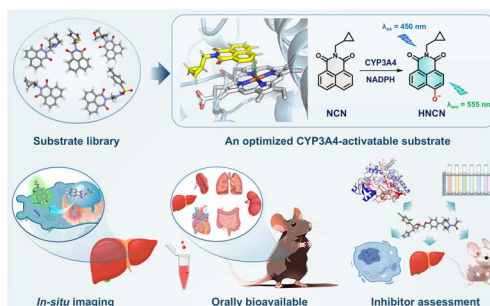
Elijah C. Gonzalez, Isabel M. de la Torre Roehl and Brian M. Stoltz\*



11386

### An optimized CYP3A4-activatable fluorogenic sensor for *in situ* functional imaging and multi-dimensional inhibitor assessment

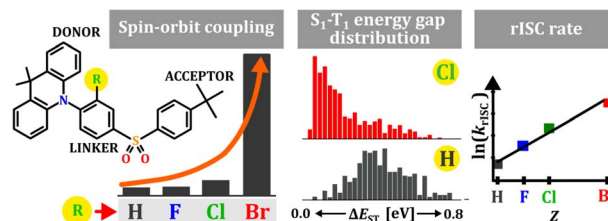
Feng Zhang, Yufan Fan, Mei Luo, Jian Huang, Bei Zhao, Lin Chen, Guanghao Zhu, Yuan Xiong, Hong Lin, Chuting Xu, Xiaodi Yang, Tony D. James\* and Guangbo Ge\*



11398

### Pursuing the holy grail of thermally activated delayed fluorescence emitters: a molecular strategy for reducing the energy gap and enhancing spin-orbit coupling

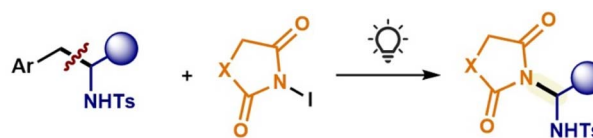
Vladyslav Ievtukhov, Antonio Prlj, Olga Ciupak, Michał Mońka and Illia E. Serdiuk\*



11413

### Visible-light-initiated metal-free $C_{sp^3}-C_{sp^3}$ to $C_{sp^3}-N$ conversion in homobenzylic sulfonamides with *N*-iodoimides

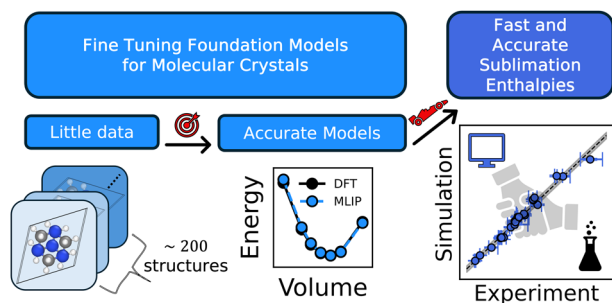
Guillermo Morales-Ortega, Estibaliz Merino and Javier Carreras\*



- $C_{sp^3}-C_{sp^3}$  to  $C_{sp^3}-N$  transformation
- *N*-centered radical
- wide functional group tolerance
- no photocatalyst



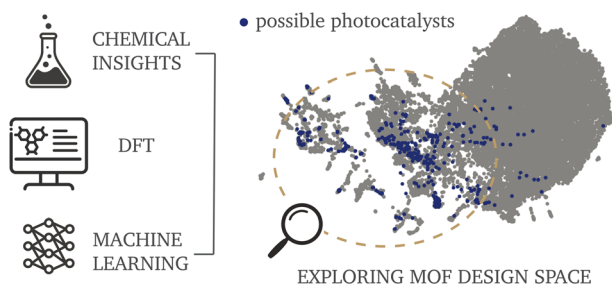
11419



### Accurate and efficient machine learning interatomic potentials for finite temperature modelling of molecular crystals

Flaviano Della Pia, Benjamin X. Shi, Venkat Kapil, Andrea Zen, Dario Alfè and Angelos Michaelides\*

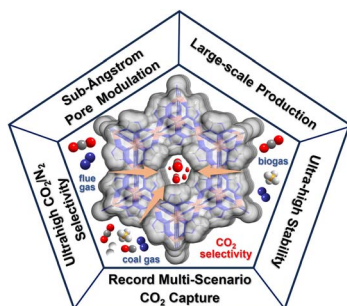
11434



### Exploring the chemical design space of metal–organic frameworks for photocatalysis

Beatriz Mourino, Sauradeep Majumdar, Xin Jin, Fergus McIlwaine, Joren Van Herck, Andres Ortega-Guerrero, Susana Garcia and Berend Smit\*

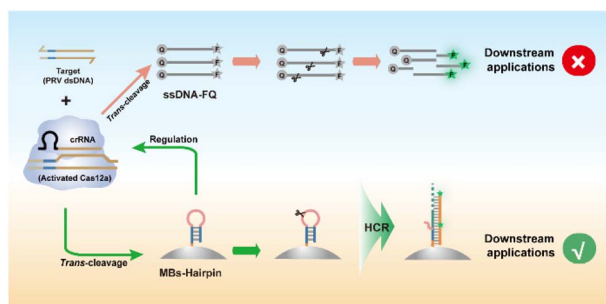
11447



### Inter-cluster-linker-absence-enabled sub-Ångstrom pore modulation in a metal–organic framework for multi-scenario CO<sub>2</sub> capture

Jia-Wen Wang, Shu-Cong Fan, Wenyu Yuan, Ying Wang and Quan-Guo Zhai\*

11456



### Regulating CRISPR/Cas12a trans-cleavage on the hairpin DNA–MB nanointerface for enhanced multiplexed sensing application

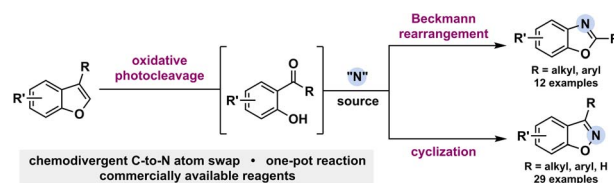
Chenxi Zhao, Lijie Du, Dike Jiang, Jing Hu\* and Xiandeng Hou\*



11464

### Chemodivergent C-to-N atom swap from benzofurans to benzisoxazoles and benzoxazoles

Ann-Sophie K. Paschke, Stefanie Schiele, Camille Pinard, Filippo Sandrini and Bill Morandi\*

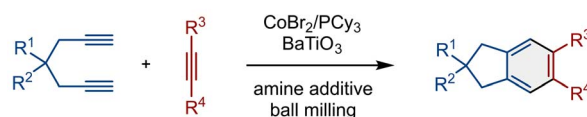


11468

### A mechanochemical [2+2+2] cycloaddition facilitated by a cobalt(II) catalyst and piezoelectric materials

Kalipada Jana, Koji Kubota\* and Hajime Ito\*

The first general mechanochemical [2+2+2] cycloaddition

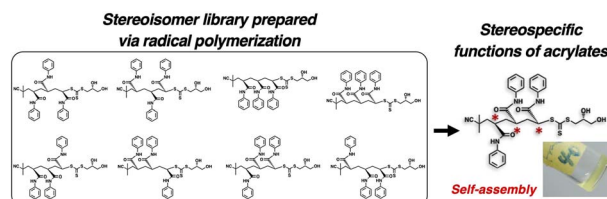


- key to success: use of piezoelectric BaTiO<sub>3</sub>-amine system as reductant
- solvent-less
- short reaction time (60 min)
- broad substrate scope

11475

### Stereoisomer library prepared via controlled radical polymerization: isolation, structural identification and discovery of stereospecific gelation behaviour of tri(N-phenyl acrylamide)

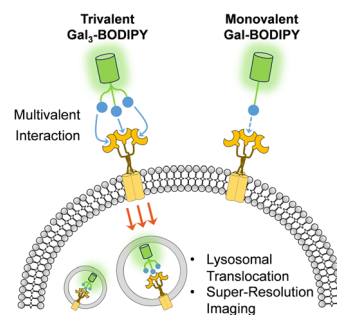
Yukiko Nagai, Hinako Iwamoto, Satoki Fukuda, Sotaro Akashi, Shota Iseri, Hayato Tada, Tomohiro Yamanaka, Konosuke Wada, Sotaro Tsuji, Toshikazu Ono, Yoshiko Miura, Tohru Taniguchi and Yu Hoshino\*



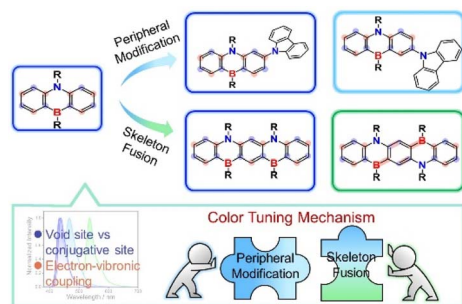
11481

### A BODIPY-tagged trivalent glycocluster for receptor-targeting fluorescence imaging of live cells

Chen Guo, Fang-Yu Si, Chen-Han Wang, Ning Wang, Xi-Le Hu, Tony D. James\*, Jia Li\*, Chengyun Wang\* and Xiao-Peng He\*



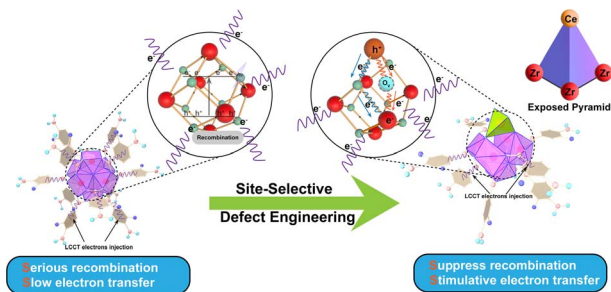
11487



### The color-tuning mechanism in multi-resonance thermally activated delayed fluorescence emitters: site effects in peripheral modification and skeleton fusion

Zicong Situ, Xingqing Li, Shengsheng Wei, Xiang Wang, Yang Li, Yan Wan, Lian Duan,\* Andong Xia\* and Zhuoran Kuang\*

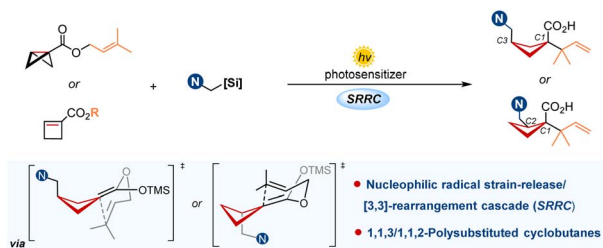
11498



### Site-selective ligand defects open up a Zr-oxo cluster electron transfer pathway for CO<sub>2</sub> photoreduction

Yuhang Qi, Yiqiang He, Yuxin Liu, Zhe Zhang, Chunguang Li, Fanchao Meng, Shiyu Wang, Xiaobo Chen, Zhan Shi\* and Shouhua Feng

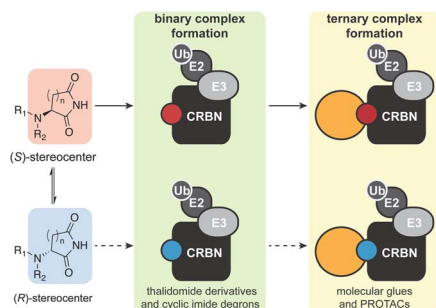
11508



### Synthesis of polysubstituted cyclobutanes through a photoredox strain-release/[3,3]-rearrangement cascade

Fangqing Zhang, Chun Xu, Zichun Zhang, Zhuang Yang, Tao Peng, Wen Shao,\* Xiaoming Feng\* and Yangbin Liu\*

11519



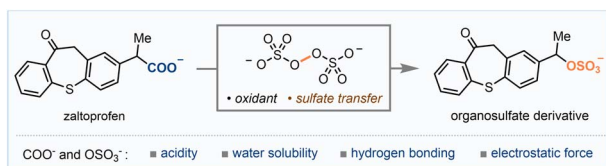
### The contribution of cyclic imide stereoisomers on cereblon-dependent activity

Yuka Amako, Saki Ichikawa, Hannah C. Lloyd, N. Connor Payne, Zhi Lin, Andrew S. Boghossian, Matthew G. Rees, Melissa M. Ronan, Jennifer A. Roth, Qian Zhu, Bogdan Budnik, Ralph Mazitschek and Christina M. Woo\*



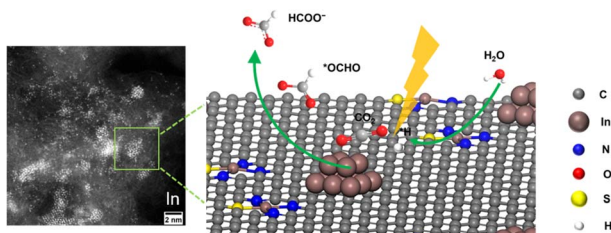


11568

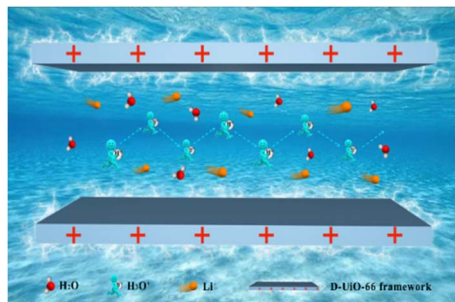
**Decarboxylative sulfation by persulfates**

Zhen Xia, Ting Deng, Chunlan Song and Jiakun Li\*

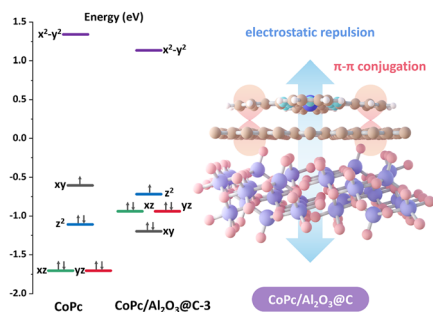
11574

**Synergistic catalysis between In single atoms and In nanoparticles for highly selective electrocatalytic CO<sub>2</sub> reduction to formate with high current densities**Yuxin Chen, Junyoung Choi, Fangkui Liang, Xinyi Tan,\*  
Yudi Chen, Jiahui Yang, Song Hong, Xin Zhang, Alex W. Robertson, Yousung Jung\* and Zhenyu Sun\*

11581

**Synergistic chaotropic effect and defect engineering promoting ultrahigh ionic conductivity in MOFs**Dongbo Liu, Xiao-Min Li,\* Junchao Jia, Xingyu Long,  
Junpeng Yan, Mengyang Xiao, Aziz Bakhtiyarovich Ibragimov and Junkuo Gao\*

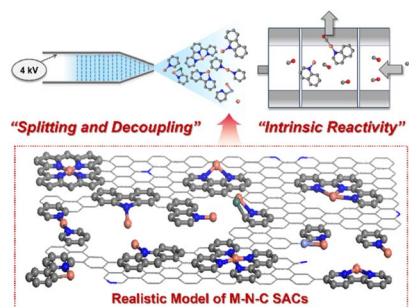
11587

**Engineering catalyst–support interactions in cobalt phthalocyanine for enhanced electrocatalytic CO<sub>2</sub> reduction: the role of graphene-skinned Al<sub>2</sub>O<sub>3</sub>**Qianqian Bai, Bingyun Ma, Le Wei, Mutian Ma,  
Zhangyi Zheng, Wei Hua, Zhenyang Jiao, Min Wang,  
Huihong Yuan, Zhihe Wei, Tao Cheng, Xiaoxing Ke,  
Jun Zhong, Fenglei Lyu,\* Zhao Deng\* and Yang Peng\*

11598

## Unraveling the local coordination effect of Cu–N–C single-atom catalysts towards CO adsorption via a gas-phase cluster model approach

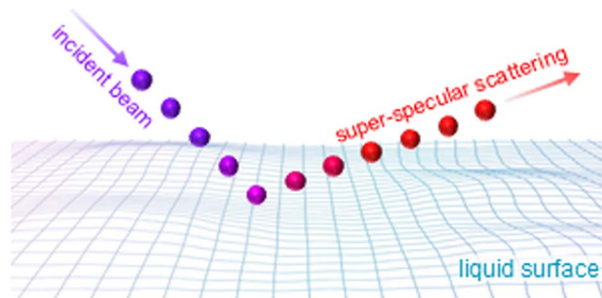
Qing Wang, Dingding Lv, Jian Zhou, Detong Kong, Shanshan Lin, Lili Zhang, Zhen-an Qiao, Yuxiao Ding\* and Xiaoyan Sun\*



11608

## Molecular beam scattering of neon from flat jets of cold salty water

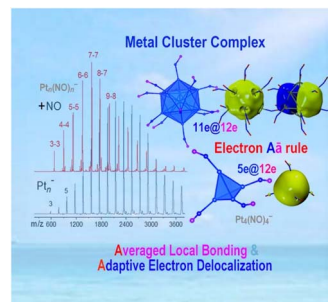
Walt Yang, Madison M. Foreman, Tiffany C. Ly, Kevin R. Wilson and Daniel M. Neumark\*



11619

## Privileged metal cluster complexes

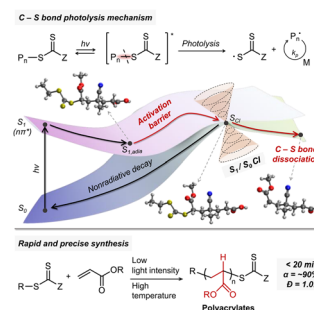
Shiquan Lin, Dan Li, Dandan Zhang, Lijun Geng, Yuhan Jia, Weizhe Wang, Longjiu Cheng,\* Shiv N. Khanna and Zhixun Luo\*



11626

## Rapid and precise synthesis of acrylic polymers driven by visible light

Changhoon Yu, Jong-Kwon Ha, Mincheol Park, Jungwook Lee, Jinho Choi, Boyoung Y. Park, Cyrille Boyer,\* Seung Kyu Min\* and Min Sang Kwon\*



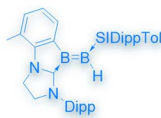
11637

## Symmetrical Cyclic Diborenes



- Isomerization from geminal to vicinal
- Geminal isomer is the most twisted diborene
- Synthesis involves spontaneous C–H borylation step

## Unsymmetrical Cyclic Diborene

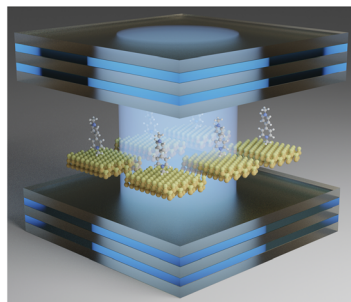


- Polarized B=B double bond
- Synthesis involves reductive C–H borylation step

## Synthesis of symmetrical and unsymmetrical cyclic diborenes via NHC-directed C–H borylation

Cornelius Mihm, Sourav Kar, Andreas Sachs, Dario Duwe, Rian D. Dewhurst and Holger Braunschweig\*

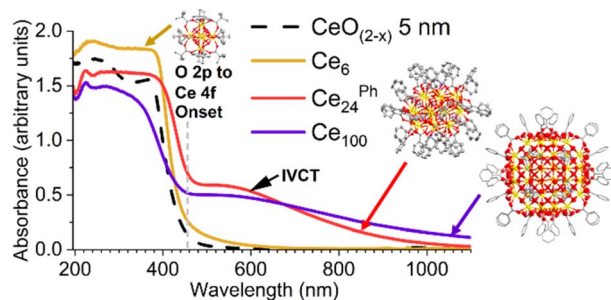
11644



## Polariton mediated electron transfer under the collective molecule–cavity coupling regime

Eric R. Koesler,\* Arkajit Mandal, Andrew J. Musser, Todd D. Krauss and Pengfei Huo\*

11659

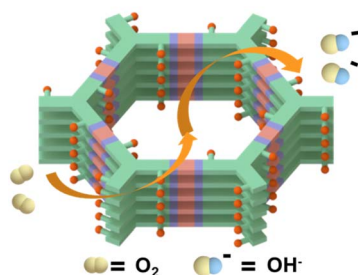


## Photoabsorption of 1–2 nm molecular Ce-oxo nanoclusters versus ceria: intervalence charge transfer but no size effects

Stephen E. Brown and Sebastian D. Pike\*

11669

## Robust imidazole-linked COFs



## Amplification effect of side group regulation via imidazolite linkages of covalent organic frameworks for efficient oxygen reduction

Mengyuan Chen, Zhiqiang Zhu, Youxin Ji,\* Xiangtao Kong, Diandian Han\* and Lipeng Zhai\*



## CORRECTIONS

11678

**Correction: Hydroxy-directed iridium-catalyzed enantioselective formal  $\beta$ -C(sp<sup>2</sup>)-H allylic alkylation of  $\alpha,\beta$ -unsaturated carbonyls**

Sankash Mitra, Rahul Sarkar, Aditya Chakrabarty and Santanu Mukherjee\*

11679

**Correction: Collective motions in the primary coordination sphere: a critical functional framework for catalytic activity of the oxygen-evolving complex of photosystem II**

Hiroshi Isobe,\* Takayoshi Suzuki, Michihiro Suga, Jian-Ren Shen and Kizashi Yamaguchi

