

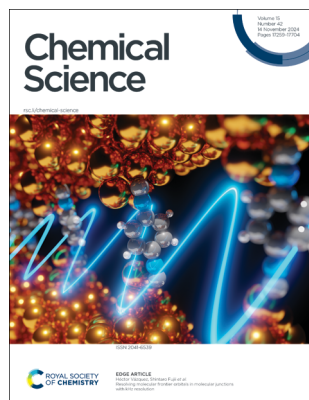
# Chemical Science

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## IN THIS ISSUE

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**Cover**  
See Héctor Vázquez, Shintaro Fujii *et al.*, pp. 17328–17336.  
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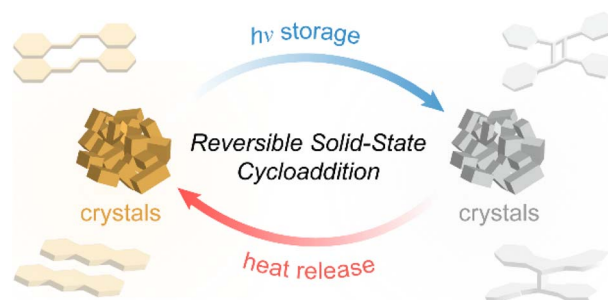
**Inside cover**  
See Bryan J. Lampkin, Joshua A. Kritzer *et al.*, pp. 17337–17347. Image reproduced by permission of Joshua A. Kritzer from *Chem. Sci.*, 2024, **15**, 17337. Illustrated by Bernadette Mary Dineen.

## PERSPECTIVES

17273

### Emerging solid-state cycloaddition chemistry for molecular solar thermal energy storage

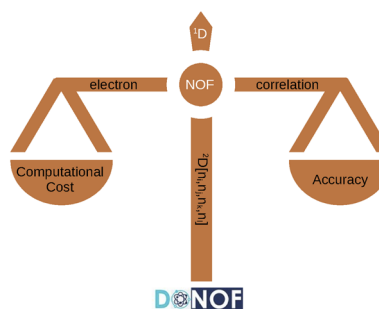
Cijil Raju, Han P. Q. Nguyen and Grace G. D. Han\*



17284

### Exploring the potential of natural orbital functionals

Mario Piris\*



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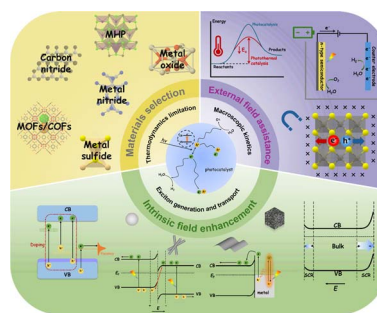
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## REVIEW

17292

## Photocatalytic overall water splitting endowed by modulation of internal and external energy fields

Wenhao Zhao, Haijun Chen, Jinqiang Zhang, Paul J. Low and Hongqi Sun\*

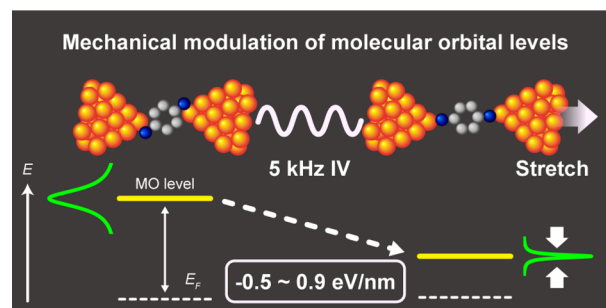


## EDGE ARTICLES

17328

## Resolving molecular frontier orbitals in molecular junctions with kHz resolution

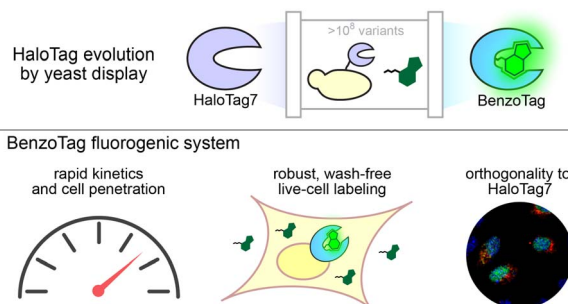
Yuji Isshiki, Enrique Montes, Tomoaki Nishino, Héctor Vázquez\* and Shintaro Fujii\*



17337

## Multiplexed no-wash cellular imaging using BenzoTag, an evolved self-labeling protein

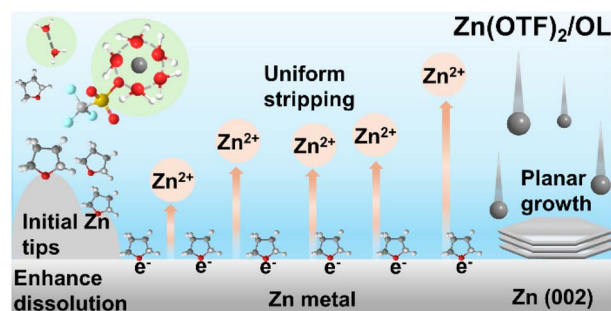
Bryan J. Lampkin,\* Benjamin J. Goldberg and Joshua A. Kritzer\*



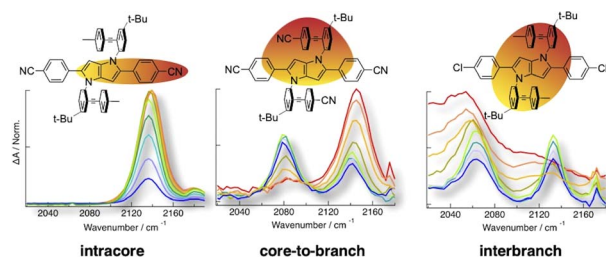
17348

## An electron-losing regulation strategy for stripping modulation towards a highly reversible Zn anode

Xinyi Wang, Liyang Liu, Zewei Hu, Chao Han, Xun Xu, Shixue Dou and Weijie Li\*



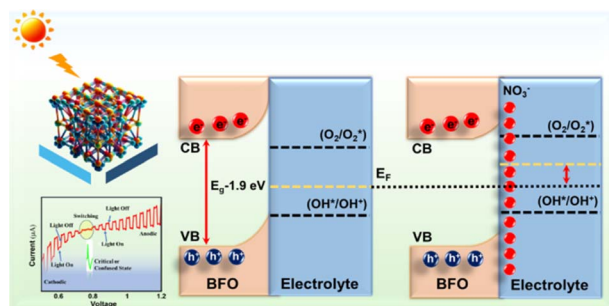
17362



### Structural and solvent modulation of symmetry-breaking charge-transfer pathways in molecular triads

Chinju Govind, Evangelos Balanikas, Gana Sanil, Daniel T. Gryko and Eric Vauthey\*

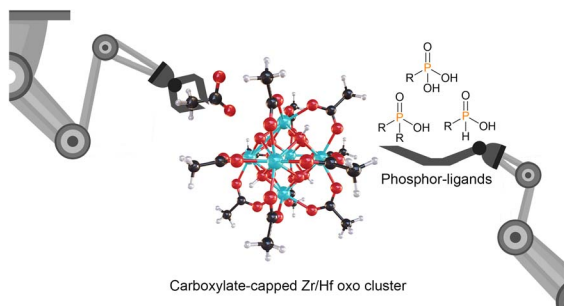
17372



### A changeable critical state for a switchable photocurrent direction via the photo-electrochemical photocurrent polarity switching effect in BiFeO<sub>3</sub> nanoparticulate films

Ajay, Jyoti Saroha and Pravin Popinand Ingole\*

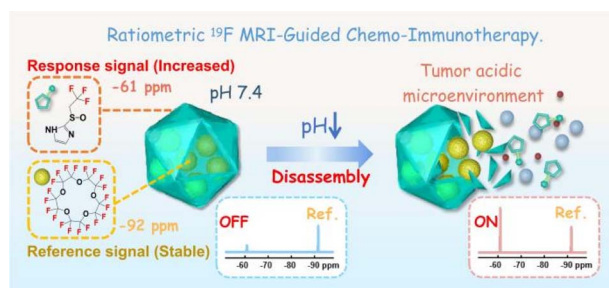
17380



### Atomically precise surface chemistry of zirconium and hafnium metal oxo clusters beyond carboxylate ligands

Ajmal Roshan Unniram Parambil, Rohan Pokratath, Muhammed Jibin Parammal, Evert Dhaene, Dietger Van den Eynden, Sandor Balog, Alessandro Prescimone, Ivan Infante, Patrick Shahgaldian and Jonathan De Roo\*

17397



### Visualization of drug release in a chemo-immunotherapy nanoplatform via ratiometric <sup>19</sup>F magnetic resonance imaging

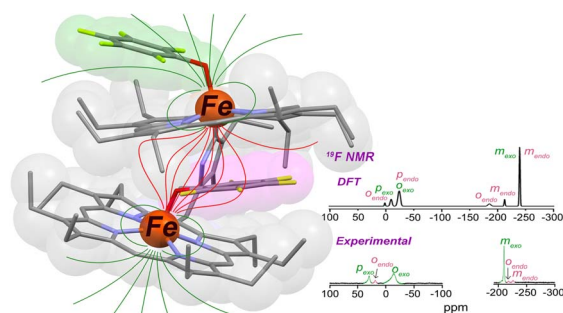
Fanqi Liu, Xindi Li, Yumin Li, Suying Xu, Chang Guo\* and Leyu Wang\*



17407

### Probing substrate binding inside a paramagnetic cavity: a NMR spectroscopy toolbox for combined experimental and theoretical investigation

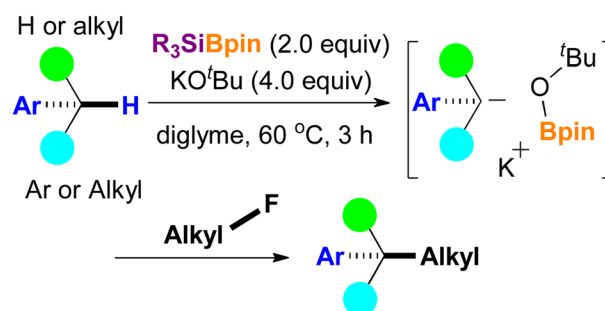
Sabyasachi Sarkar, Chang-Quan Wu, Santanu Manna, Deepannita Samanta, Peter P.-Y. Chen\* and Sankar Prasad Rath\*



17418

### A silylboronate-mediated strategy for cross-coupling of alkyl fluorides with aryl alkanes: mechanistic insights and scope expansion

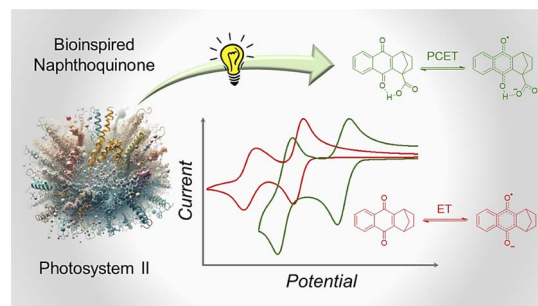
Jun Zhou, Zhengyu Zhao, Tatsuki Kiyono, Ayaka Matsuno, Jorge Escorihuela and Norio Shibata\*



17425

### The role of an intramolecular hydrogen bond in the redox properties of carboxylic acid naphthoquinones

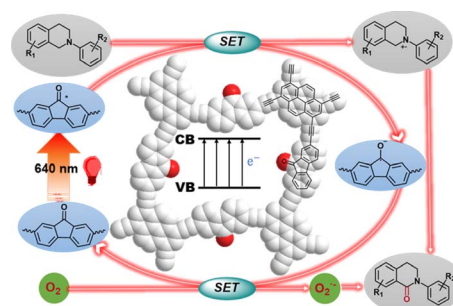
Walter D. Guerra, Emmanuel Odella, Kai Cui, Maxim Secor, Rodrigo E. Dominguez, Edwin J. Gonzalez, Thomas A. Moore, Sharon Hammes-Schiffer\* and Ana L. Moore\*



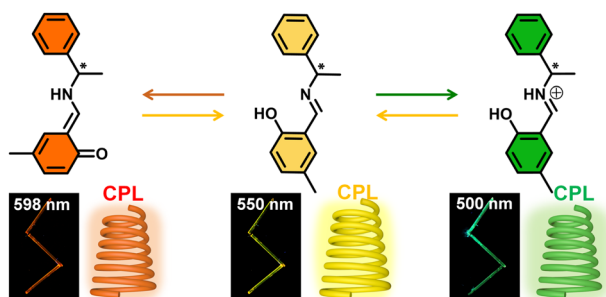
17435

### Ketone-functionalized conjugated organic polymers boost red-light-driven molecular oxygen-mediated oxygenation

Hao Zhang,\* Tingting Yuan, Nursaya Zhumabay, Zhipeng Ruan,\* Hai Qian\* and Magnus Rueping\*



17444

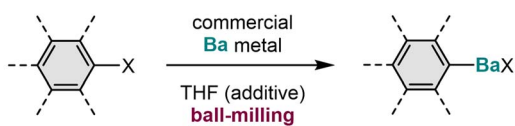


### Flexible organic crystals with multi-stimuli-responsive CPL for broadband multicolor optical waveguides

Xiuhong Pan, Linfeng Lan and Hongyu Zhang\*

17453

### Mechanochemical generation of organobarium nucleophiles

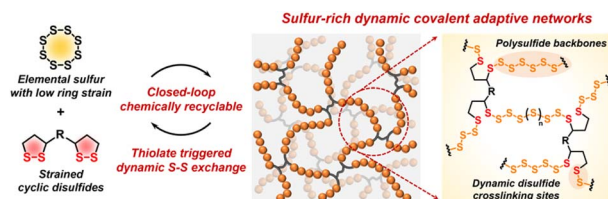


- commercial Ba metal can be used
- simple synthetic procedures
- rapid development of new reactions with organobariums

### Mechanochemical generation of aryl barium nucleophiles from unactivated barium metal

Koji Kubota,\* Sota Kawamura, Julong Jiang, Satoshi Maeda and Hajime Ito\*

17460

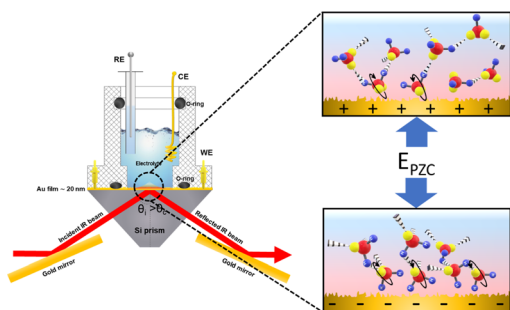


- ✓ Tunable cyclic disulfide comonomers
- ✓ High sulfur content (40 ~ 70wt%)
- ✓ Mechanical robustness
- ✓ Reprocessability
- ✓ Chemical recyclability
- ✓ NIR optical transparency

### Closed-loop chemically recyclable covalent adaptive networks derived from elementary sulfur

Chen-Yu Shi, Xiao-Ping Zhang, Qi Zhang, Meng Chen, He Tian and Da-Hui Qu\*

17469



### Water at electrode–electrolyte interfaces: combining HOD vibrational spectra with *ab initio*-molecular dynamics simulations

Pavithra Gunasekaran, Xianglong Du, Andrew Burley, Jiabo Le, Jun Cheng and Angel Cuesta\*

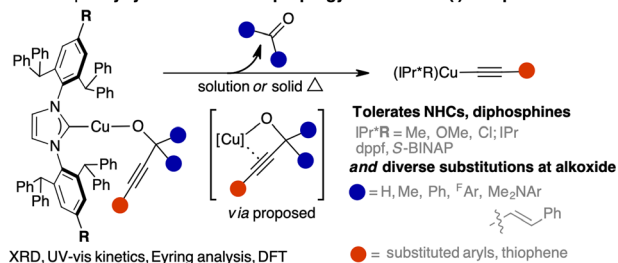


17481

## Direct observation of $\beta$ -alkynyl eliminations from unstrained propargylic alkoxide Cu(I) complexes by C–C bond cleavage

Ba L. Tran,<sup>\*</sup> Jack T. Fuller, III, Jeremy D. Erickson, Bojana Ginovska<sup>\*</sup> and Simone Raugel<sup>\*</sup>

### General $\beta$ -alkynyl eliminations of propargylic alkoxide Cu(I) complexes



17490

## Bromine radical release from a nickel-complex facilitates the activation of alkyl boronic acids: a boron selective Suzuki–Miyaura cross coupling

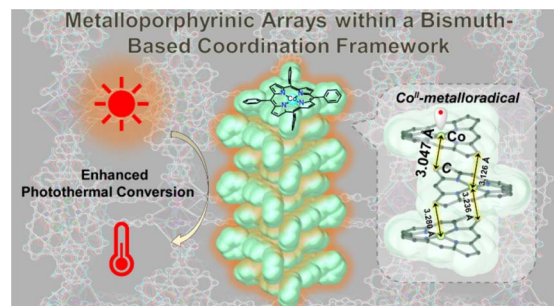
Monica Oliva, Serena Pillitteri, Johannes Schörghenheimer, Riku Saito, Erik V. Van der Eycken and Upendra K. Sharma<sup>\*</sup>



17498

## Boosting photothermal conversion through array aggregation of metalloporphyrins in bismuth-based coordination frameworks

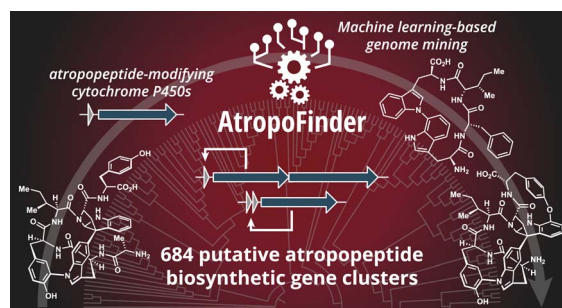
Liang He, Jing He, Er-Xia Chen<sup>\*</sup> and Qipu Lin<sup>\*</sup>



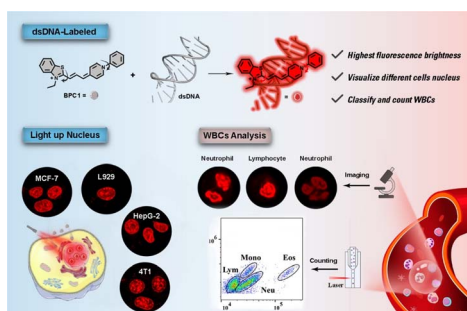
17506

## Exploration, expansion and definition of the atropopeptide family of ribosomally synthesized and posttranslationally modified peptides

Friederike Biermann, Bin Tan, Milena Breitenbach, Yuya Kakumu, Pakjira Nanudorn, Yoana Dimitrova, Allison S. Walker, Reiko Ueoka and Eric J. N. Helfrich<sup>\*</sup>



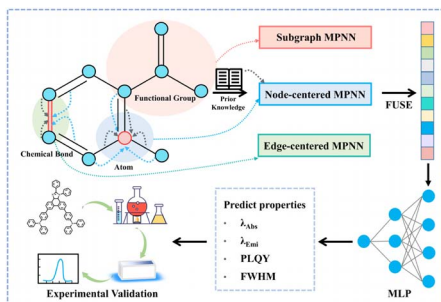
17524



### Next-generation red ultra-bright fluorescent dyes for nuclear imaging and peripheral blood leukocytes sorting

Zipeng Li, Zheng Liu, Ding Yu, Qichao Yao, Wanying Ma, Changyu Zhang, Jiangli Fan\* and Xiaojun Peng

17533



### Enhancing chemistry-intuitive feature learning to improve prediction performance of optical properties

Ming Sun, Caixia Fu, Haoming Su, Ruyue Xiao, Chaojie Shi, Zhiyun Lu\* and Xuemei Pu\*

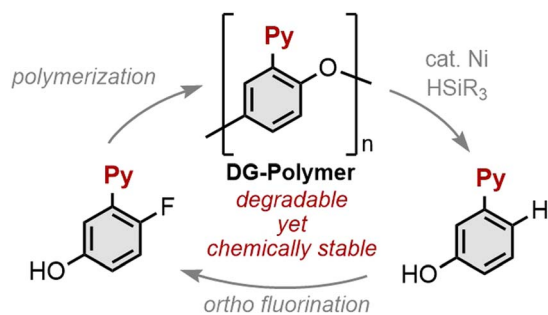
17547



### Metal-organic frameworks with two different-sized aromatic ring-confined nanotraps for benchmark natural gas upgrade

Shu-Yi Li, Ying-Ying Xue, Jia-Wen Wang, Hai-Peng Li, Jiao Lei, Hong-Juan Lv, Xianhui Bu,\* Peng Zhang, Ying Wang, Wen-Yu Yuan and Quan-Guo Zhai\*

17556



### Controlled degradation of chemically stable poly(aryl ethers) via directing group-assisted catalysis

Satoshi Ogawa, Hiroki Morita, Yu-I. Hsu, Hiroshi Uyama\* and Mamoru Tobisu\*

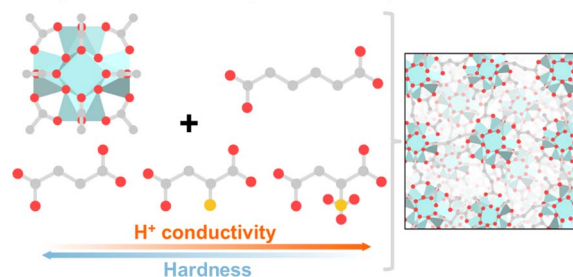


17562

### Systematic design and functionalisation of amorphous zirconium metal–organic frameworks

Nattapol Ma,\* Soracha Kosasang, Jennifer Theissen, Nick Gys, Tom Hauffman, Ken-ichi Otake, Satoshi Horike and Rob Ameloot\*

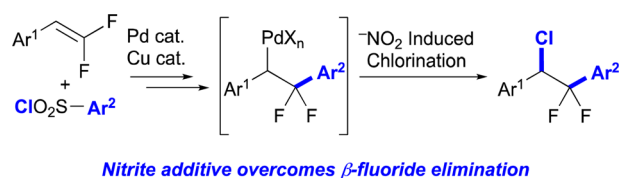
### Systematic design of amorphous MOFs



17571

### Palladium and copper co-catalyzed chloro-arylation of *gem*-difluorostyrenes – use of a nitrite additive to suppress $\beta$ -F elimination

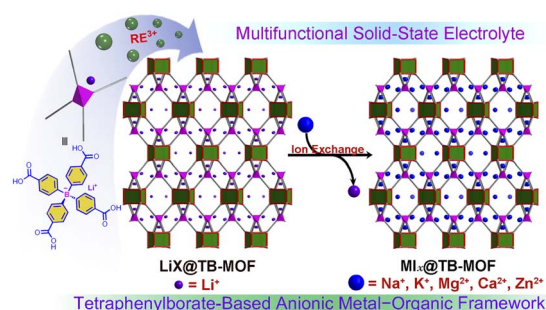
Andrew J. Intelli, Coriantumr Z. Wayment, Ryan T. Lee, Kedong Yuan and Ryan A. Altman\*



17579

### A tetraphenylborate-based anionic metal–organic framework as a versatile solid electrolyte for fast $\text{Li}^+$ , $\text{Na}^+$ , $\text{K}^+$ , $\text{Mg}^{2+}$ , $\text{Ca}^{2+}$ , and $\text{Zn}^{2+}$ transportation

Qingchun Xia,\* Kaixin Han, Xuxiao Ma, Pengtao Qiu,\* Zhiyong Li and Xuenian Chen\*



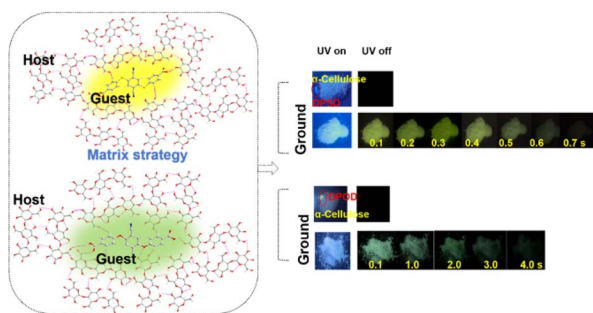
17590

### Preparation of superstructured comb polymers based on tadpole-shaped single-chain nanoparticles

Yangjing Chen, Zhiyu Hu, Zhigang Shen, Xiaoqiang Xue and Hongting Pu\*



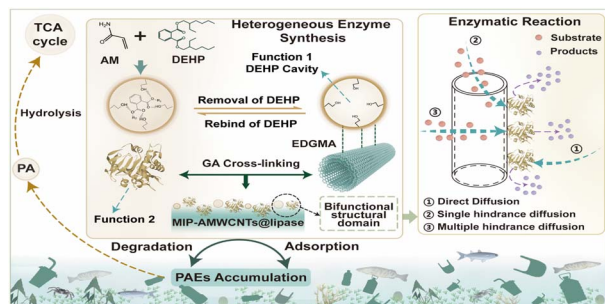
17600



### Long-persistent luminescence by host–guest Förster resonance energy transfer

Hui-Li Sun, Qiang-Sheng Zhang, Zhong-Hao Wang, Yan-Ting Huang and Mei Pan\*

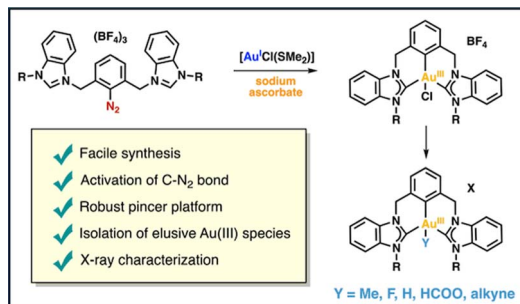
17608



### A carbon-based bifunctional heterogeneous enzyme: toward sustainable pollution control

Yuting Sun, Ming Guo,\* Shengnan Hu, Yankun Jia, Wenkai Zhu,\* Yusuke Yamauchi\* and Chaohai Wang\*

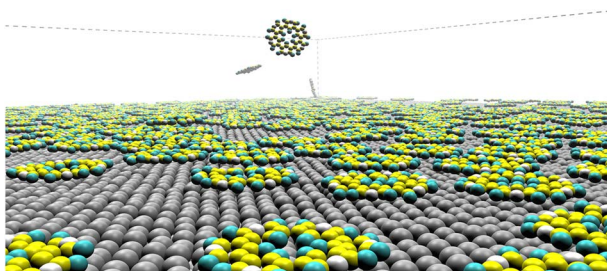
17618



### CCC-NHC Au(III) pincer complexes as a reliable platform for isolating elusive species

Hugo Valdés,\* Nora Alpuente, Pedro Salvador, A. Stephen K. Hashmi\* and Xavi Ribas\*

17629



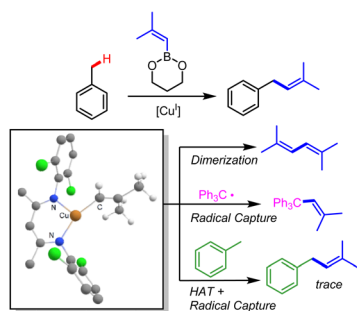
### Growth of two-dimensional covalent organic frameworks on substrates: insight from microsecond atomistic simulations

Zilin Wang, Hong Du, Austin M. Evans,\* Xiaojuan Ni, Jean-Luc Bredas\* and Haoyuan Li\*



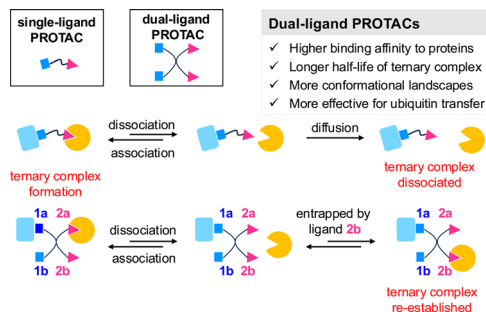


17685

Copper catalyzed benzylic  $sp^3$  C–H alkenylation

Ting-An Chen, Richard J. Staples and Timothy H. Warren\*

17691

Dual-ligand PROTACs mediate superior target protein degradation *in vitro* and therapeutic efficacy *in vivo*

Yong Chen, Zihan Xia, Ujjwal Suwal, Pekka Rappu, Jyrki Heino, Olivier De Wever\* and Bruno G. De Geest\*

