

# 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

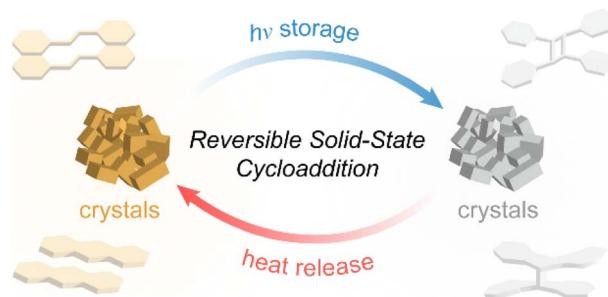
See Bryan J. Lampkin,  
Joshua A. Kritzer et al.,  
pp. 17337–17347. Image  
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Joshua A. Kritzer from *Chem.  
Sci.*, 2024, 15, 17337. Illustrated  
by Bernadette Mary Dineen.

## PERSPECTIVES

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

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



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### Exploring the potential of natural orbital functionals

Mario Piris\*



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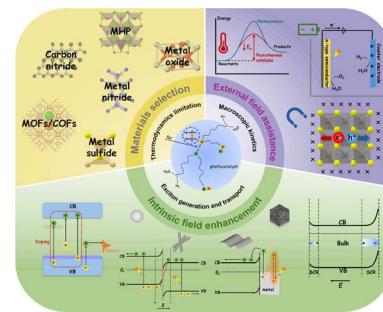


## REVIEW

17292

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

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

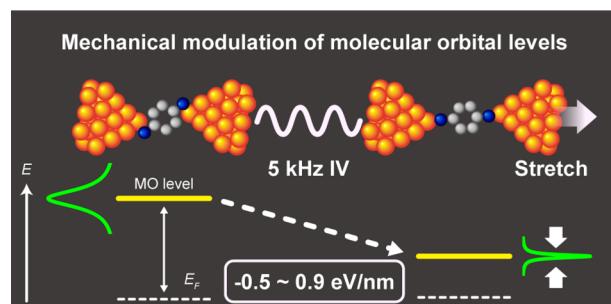


## EDGE ARTICLES

17328

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

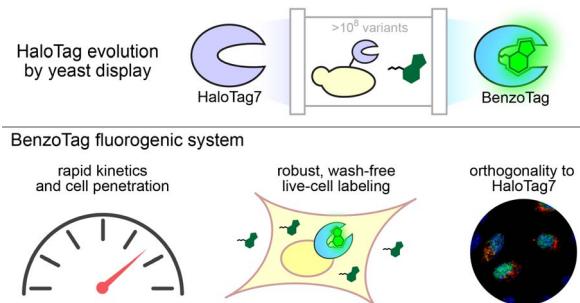
Yuji Isshiki, Enrique Montes, Tomoaki Nishino, Héctor Vázquez\* and Shintaro Fujii\*



17337

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

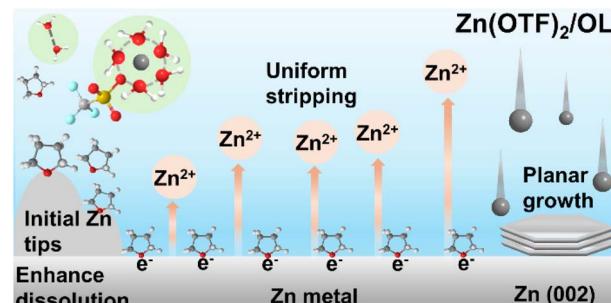
Bryan J. Lampkin,\* Benjamin J. Goldberg and Joshua A. Kritzer\*



17348

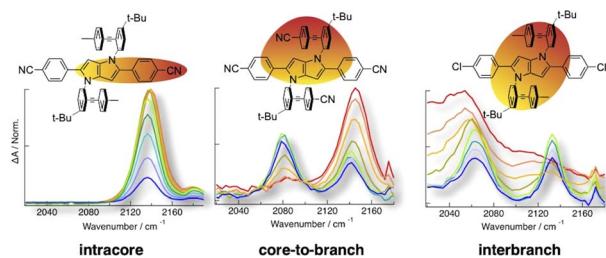
**An electron-losing regulation strategy for stripping modulation towards a highly reversible Zn anode**

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



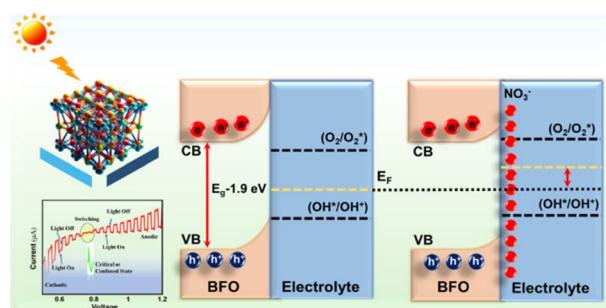
## EDGE ARTICLES

17362

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

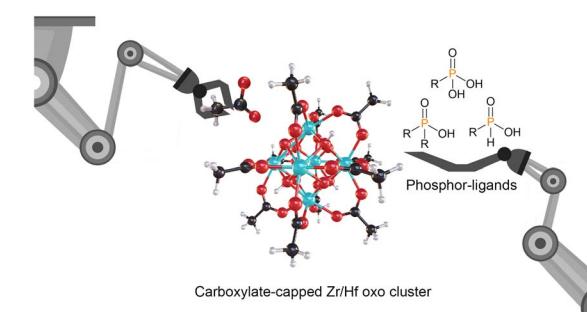
Chinju Govind, Evangelos Balanikas, Gana Sanil, Daniel T. Gryko and Eric Vauthey\*

17372

**A changeable critical state for a switchable photocurrent direction via the photo-electrochemical photocurrent polarity switching effect in  $\text{BiFeO}_3$  nanoparticulate films**

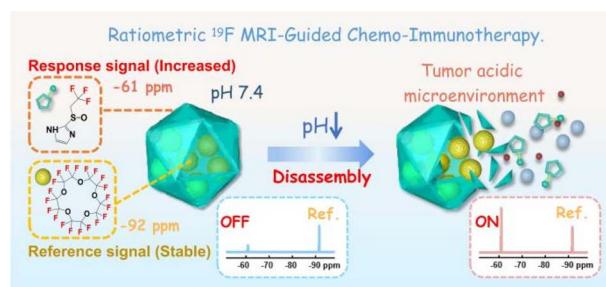
Ajay, Jyoti Saroha and Pravin Popinand Ingole\*

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 nanoplateform via ratiometric  $^{19}\text{F}$  magnetic resonance imaging**

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

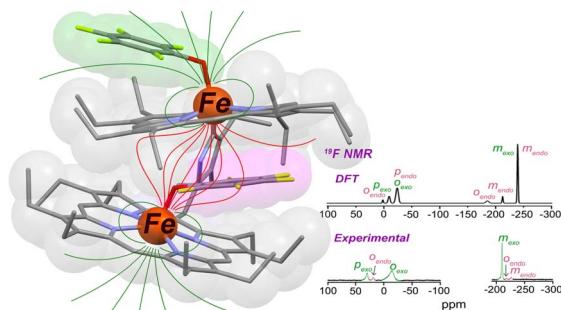


## EDGE ARTICLES

17407

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

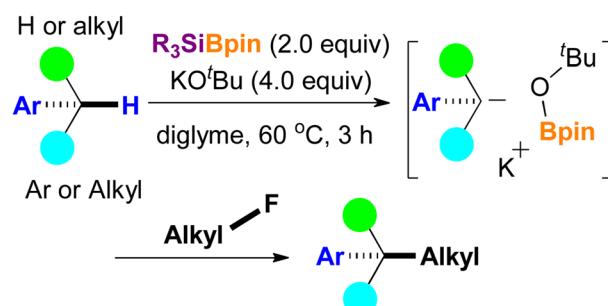
Sabyasachi Sarkar, Chang-Quan Wu, Santanu Manna, Deepannita Samanta, Peter P.-Y. Chen\* and Sankar Prasad Rath\*



17418

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

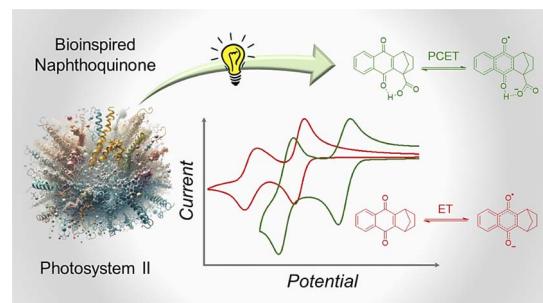
Jun Zhou, Zhengyu Zhao, Tatsuki Kiyono, Ayaka Matsuno, Jorge Escorihuela and Norio Shibata\*



17425

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

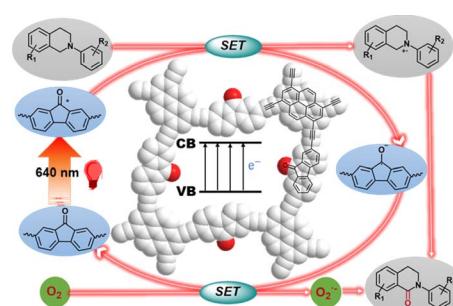
Walter D. Guerra, Emmanuel Odella, Kai Cui, Maxim Secor, Rodrigo E. Dominguez, Edwin J. Gonzalez, Thomas A. Moore, Sharon Hammes-Schiffer\* and Ana L. Moore\*



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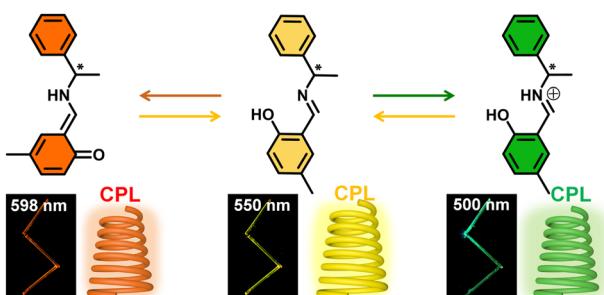
**Ketone-functionalized conjugated organic polymers boost red-light-driven molecular oxygen-mediated oxygenation**

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



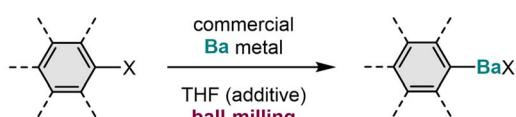
## EDGE ARTICLES

17444

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

Xiuhong Pan, Linfeng Lan and Hongyu Zhang\*

17453

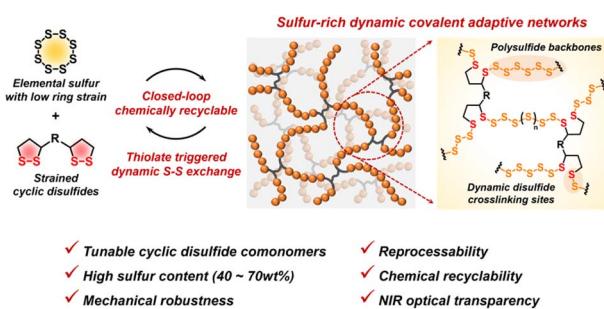
**Mechanochemical generation of organobarium nucleophiles**

- 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**

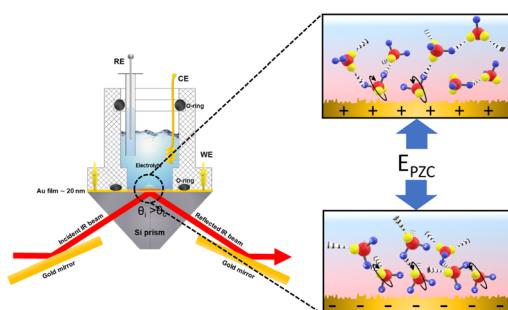
Koji Kubota,\* Sota Kawamura, Julong Jiang, Satoshi Maeda and Hajime Ito\*

17460

**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**

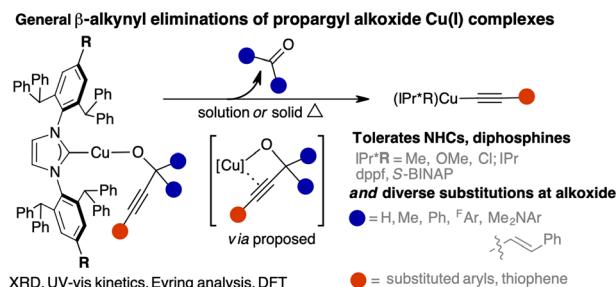
Pavithra Gunasekaran, Xianglong Du, Andrew Burley, Jiabo Le, Jun Cheng and Angel Cuesta\*

## EDGE ARTICLES

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

Ba L. Tran,\* Jack T. Fuller, III, Jeremy D. Erickson, Bojana Ginovska\* and Simone Raugei\*



17490

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

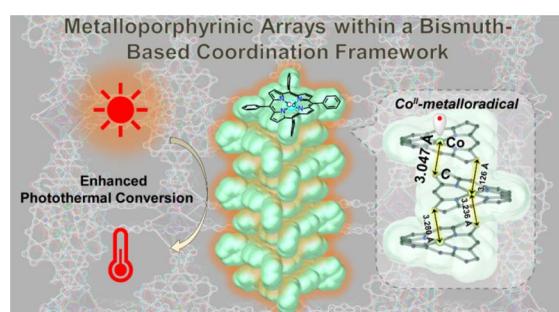
Monica Oliva, Serena Pillitteri, Johannes Schörgenhummer, Riku Saito, Erik V. Van der Eycken and Upendra K. Sharma\*



17498

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

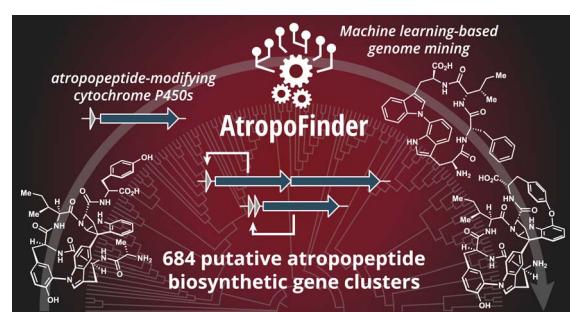
Liang He, Jing He, Er-Xia Chen\* and Qipu Lin\*



17506

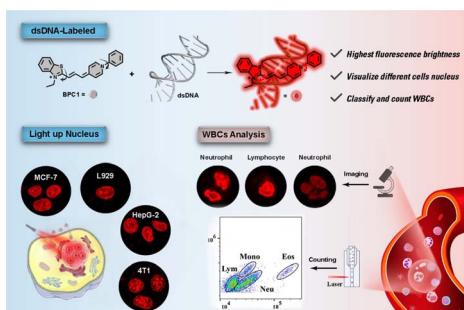
**Exploration, expansion and definition of the atropopeptide family of ribosomally synthesized and posttranslationally modified peptides**

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



## EDGE ARTICLES

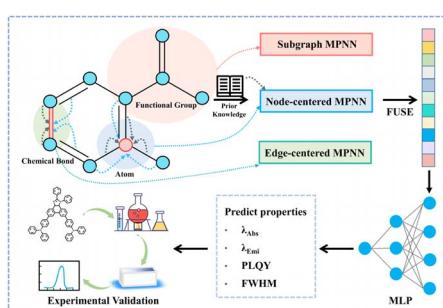
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### Next-generation red ultra-bright fluorescent dyes for nuclear imaging and peripheral blood leukocytes sorting

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

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### 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\*

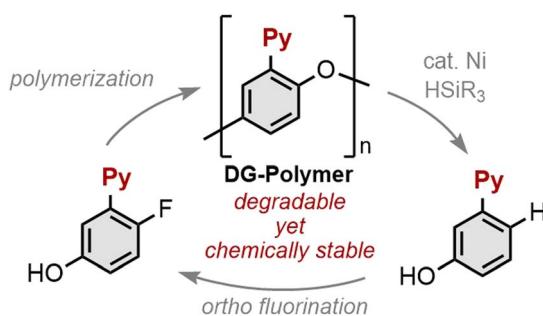
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### Metal–organic frameworks with two different-sized aromatic ring-confined nanotrap for benchmark natural gas upgrade

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\*

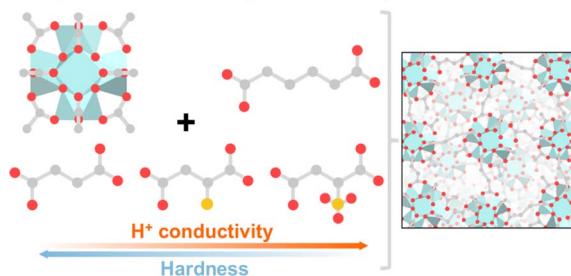


## EDGE ARTICLES

17562

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

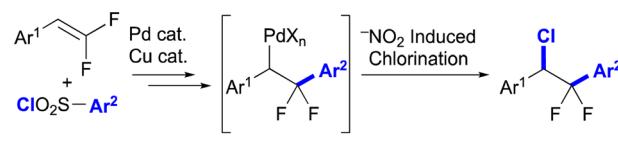
Nattapol Ma,\* Soracha Kosasang, Jennifer Theissen, Nick Gys, Tom Hauffman, Ken-ichi Otake, Satoshi Horike and Rob Ameloot\*

**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**

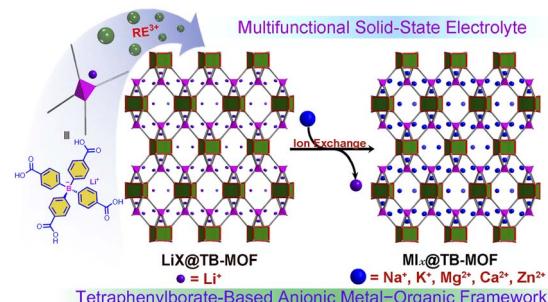
Andrew J. Intelli, Coriantumr Z. Wayment, Ryan T. Lee, Kedong Yuan and Ryan A. Altman\*

*Nitrite additive overcomes  $\beta$ -fluoride elimination*

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

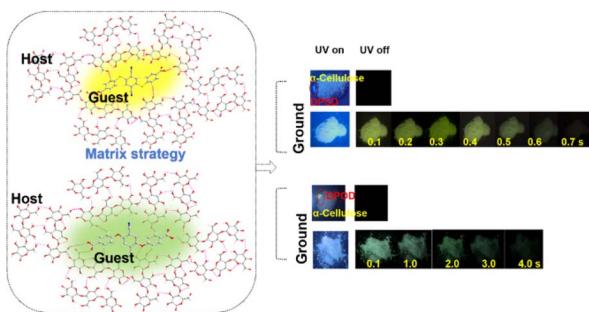
**Preparation of superstructured comb polymers based on tadpole-shaped single-chain nanoparticles**

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



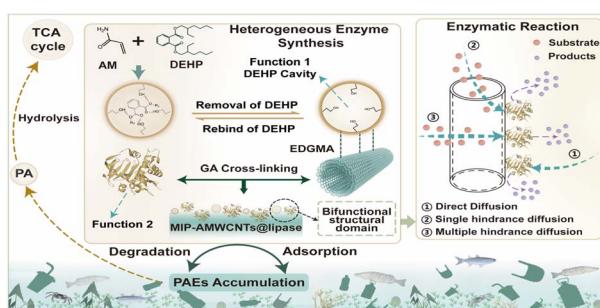
## EDGE ARTICLES

17600

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

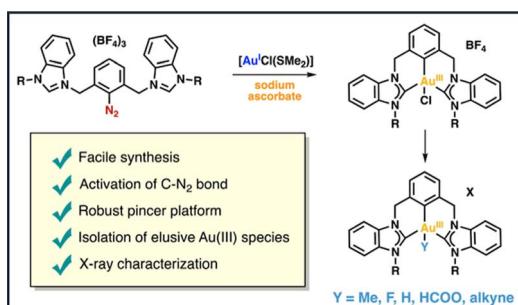
Hui-Li Sun, Qiang-Sheng Zhang, Zhong-Hao Wang, Yan-Ting Huang and Mei Pan\*

17608

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

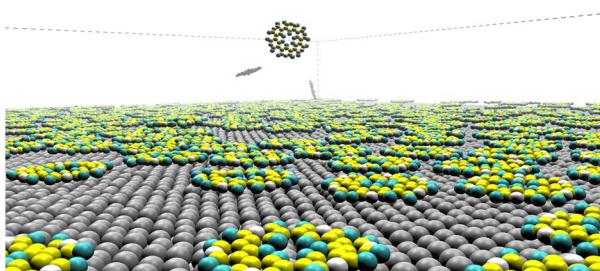
Yuting Sun, Ming Guo,\* Shengnan Hu, Yankun Jia, Wenkai Zhu,\* Yusuke Yamauchi\* and Chaohai Wang\*

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**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\*

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**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\*

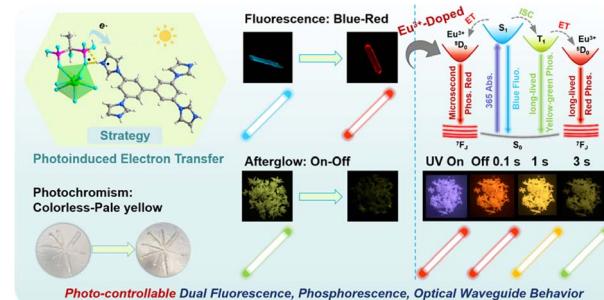


## EDGE ARTICLES

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**A photoinduced electron-transfer strategy for switchable fluorescence and phosphorescence in lanthanide-based coordination polymers**

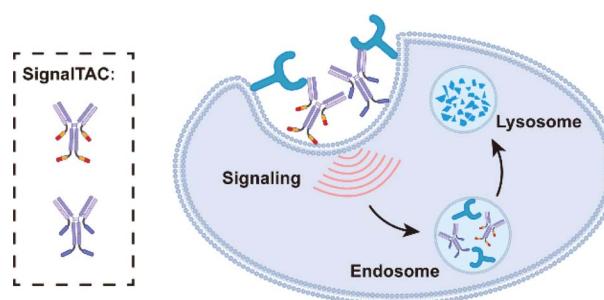
Yu-Juan Ma, Fei Xu, Xin-Ye Ren, Fan-Yao Chen, Jie Pan, Jin-Hua Li,\* Song-De Han\* and Guo-Ming Wang\*



17652

**Lysosome–targeting chimeras containing an endocytic signaling motif trigger endocytosis and lysosomal degradation of cell-surface proteins**

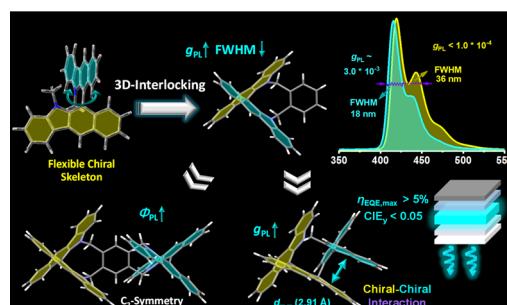
Tong Fang, Zhenting Zheng, Na Li, Yishu Zhang, Jing Ma, Chengyu Yun and Xiaoqing Cai\*



17663

**Enhanced chiroptical activity for narrow deep-blue emission in axial chiral frameworks via three-dimensional interlocking**

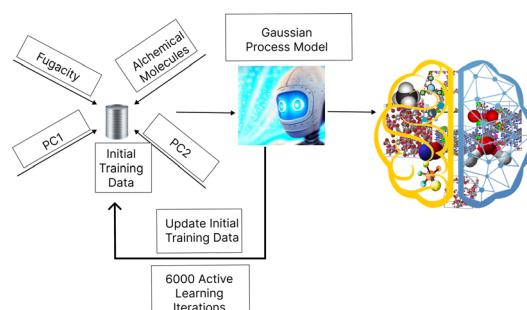
Xuechao Mo, Guohao Chen, Yulan Li, Biao Xiao, Xuefeng Chen, Xiaojun Yin\* and Chuluo Yang\*



17671

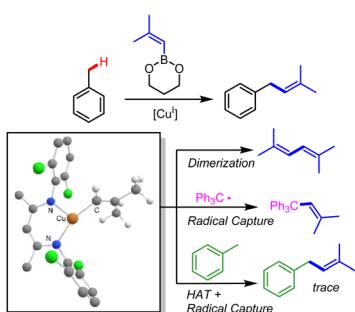
**Active learning of alchemical adsorption simulations; towards a universal adsorption model**

Etinosa Osaro, Fernando Fajardo-Rojas, Gregory M. Cooper, Diego Gómez-Gualdrón and Yamil J. Colón\*



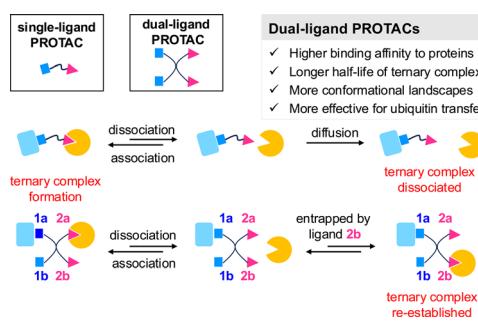
## EDGE ARTICLES

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**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\*

