

# Chemical Science

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## IN THIS ISSUE

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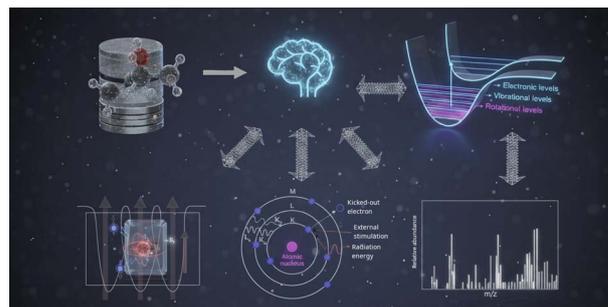
**Inside cover**  
See Andreas Brunschweiler *et al.*, pp. 21781–21790. Image reproduced by permission of Johannes Bingold, Cornelia Janda and Andreas Brunschweiler from *Chem. Sci.*, 2025, **16**, 21781. Created in part with Google Gemini.

## PERSPECTIVE

21660

### Machine learning spectroscopy to advance computation and analysis

Julia Westermayr\* and P. Marquetand



## REVIEWS

21677

### Can single-atom precision rewire the electrochemical logic of Li–S chemistry? A comprehensive review of single-atom catalysts as agents of precise modulation

Yue Wang, Haobin Song, Nan Zhao, Xi Cheng, Dong-Sheng Li and Hui Ying Yang\*



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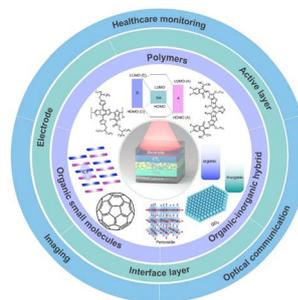
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## REVIEWS

21705

### High-performance organic semiconductor near-infrared and shortwave-infrared photodetectors: a materials and device roadmap

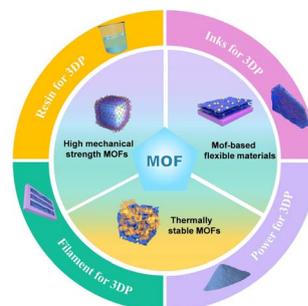
Hongyu Tan, Xianshuo Wu, Suhao Hu, Yiwen Ren, Yuhan Du, Qiang Zhao, Lingjie Sun,\* Fangxu Yang\* and Wenping Hu



21745

### Bridging MOF properties to 3D printing: a framework for electrochemical energy storage architectures with synergistic porosity-ion dynamics

Chenfei Zhou, Huijie Zhou,\* Xinyu Qin,\* Shunyu Gu, Mengyao Zhang, Jifan Chen, Lingfeng Zhai and Huan Pang\*

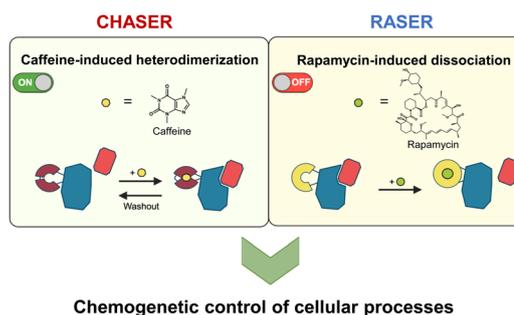


## EDGE ARTICLES

21774

### Reprogramming chemically induced dimerization systems with genetically encoded nanobodies

Tianlu Wang, Tatsuki Nonomura, Mingguang Cui, Tien-Hung Lan, Pauline X. Cai, Lian He\* and Yubin Zhou\*



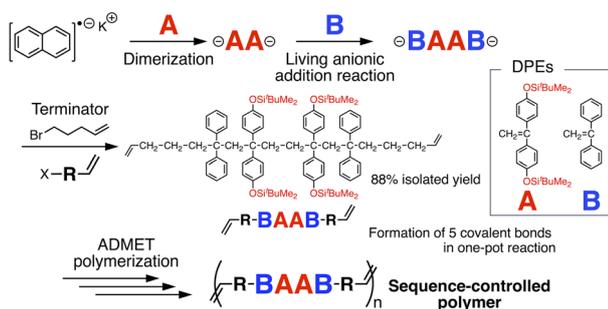
21781

### Aggregation of DNA oligomers with a neutral polymer facilitates DNA solubilization in organic solvents for DNA-encoded chemistry

Johannes Bingold, Erik Mafenbayer, Wibke Langenkamp, Lisa Liang, Chun Zhang, Malte Mildner, Julia Isabel Bahner, Mohamed Akmal Marzouk, Bettina Böttcher, Ann-Christin Pöppler, Ralf Weberskirch and Andreas Brunschweiler\*



21791

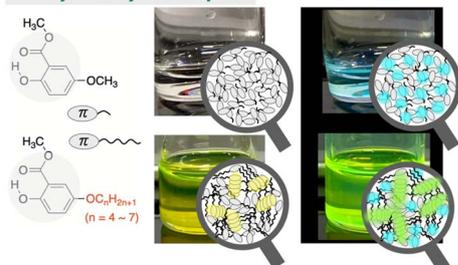


### One-pot synthesis of sequence-controlled macromonomers *via* living anionic addition reaction and subsequent acyclic diene metathesis polymerization

Tomohiko Nishijima, Kazuki Takahata, Raita Goseki, Chihiro Homma, Shigeki Kuwata and Takashi Ishizone\*

21797

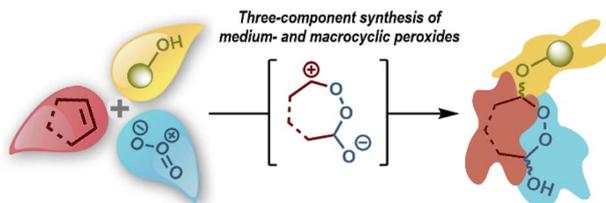
### Methyl Salicylate Liquids



### Harnessing inhomogeneous $\pi$ -aggregates: a new path to optical modulation in methyl salicylate-based solvent-free liquids

Kei Kobayashi, Ken-ichi Sakai,\* Tomoyuki Akutagawa and Takashi Nakanishi

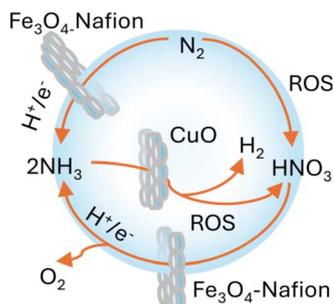
21806



### "Trading" a $C=C$ moiety for four $C-O$ bonds and a peroxide: combining ozone and $O$ -nucleophiles for peroxidative ring expansion of cycloalkenes into medium-sized 1,2-dioxacycloalkanes

Roman A. Budekhin, Dmitri I. Fomenkov, Alexander O. Ustyuzhanin, Darya Yu. Sliguzova, Ksenia V. Skokova, Vera A. Vil', Igor V. Alabugin\* and Alexander O. Terent'ev\*

21815



### The air–water interfacial nitrogen cycle produces irrigatable-level ammonium nitrate

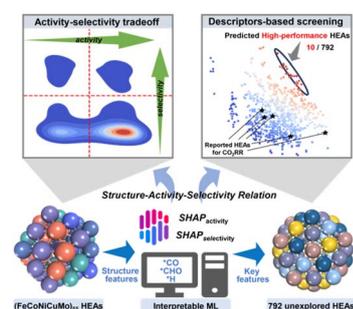
Xiaowei Song, Chanbasha Basheer,\* Jinheng Xu and Richard N. Zare\*



21825

## Deciphering the structure–activity–selectivity relationship of high-entropy alloys for CO<sub>2</sub> reduction via interpretable machine learning

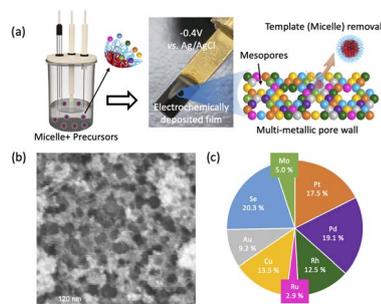
Jinxin Sun, Xiaokang Xu, Yuqing Mao, Anjie Chen, Shu Wang, Li Shi,\* Chongyi Ling,\* Jinlan Wang\* and Xiuyun Zhang\*



21836

## Electrochemical deposition of mesoporous high-entropy Pt–Pd–Rh–Ru–Cu–Au–Se–Mo films using polymeric micelle templating

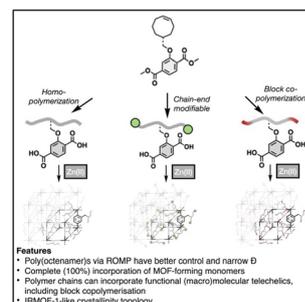
Yoto Saso, Yunqing Kang,\* Lei Fu, Kotaro Yagi, Jungmok You, Yusuke Asakura and Yusuke Yamauchi\*



21842

## Tailoring polymer-metal–organic frameworks (polyMOFs) using telechelic poly(octenamer)s

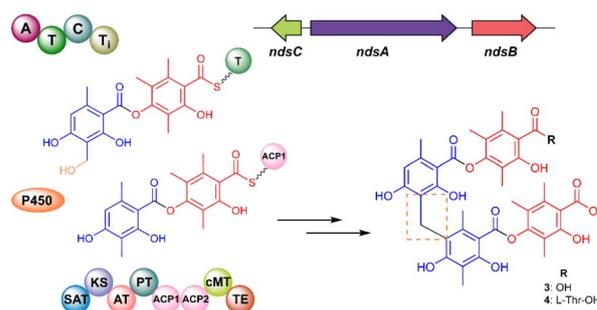
Prantik Mondal, Debobroto Sensharma and Seth M. Cohen\*



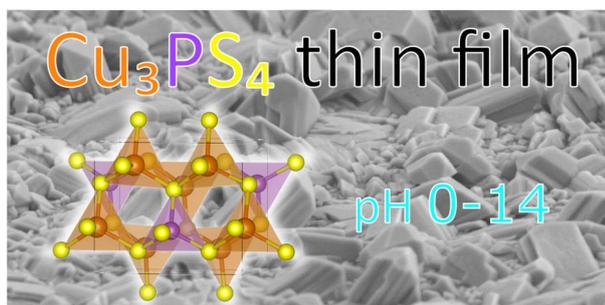
21852

## Heterologous expression of an *in planta*-upregulated gene cluster in the wheat pathogen *Parastagonospora nodorum* establishes the biosynthesis of methylene-bridged depsides

Hera T. Nguyen, Nicolau Sbaraini, Joe Bracegirdle, Luke Smithers, Stephen A. Moggach, Daniel Vuong, Ernest Lacey, Peter S. Solomon, Joel Haywood, Andrew M. Piggott\* and Yit-Heng Chooi\*



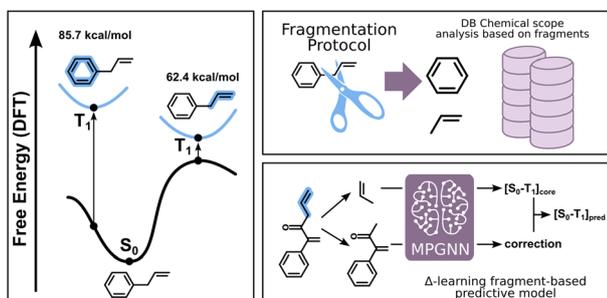
21862



## Large-area thin-film synthesis of photoactive $\text{Cu}_3\text{PS}_4$ thiophosphate semiconductor with 0–14 pH stability range

Lena A. Mittmann,<sup>\*</sup> Javier Sanz Rodrigo, Eugène Bertin, Giulia Dalmonte, Jean-Claude Grivel, Ivano E. Castelli and Andrea Crovetto<sup>\*</sup>

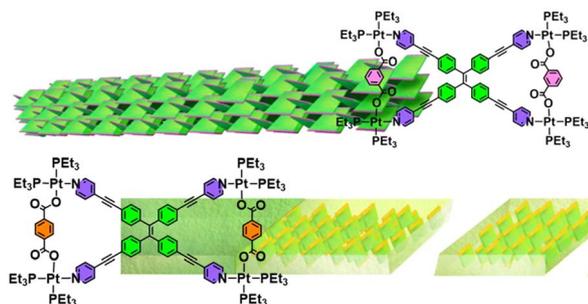
21874



## A fragment based approach towards curating, comparing and developing machine learning models applied in photochemistry

Raúl Pérez-Soto, Mihai V. Popescu, Sabari Kumar, Leticia A. Gomes, Changyeob Lee, Elijah Shore, Steven A. Lopez,<sup>\*</sup> Robert S. Paton<sup>\*</sup> and Seonah Kim<sup>\*</sup>

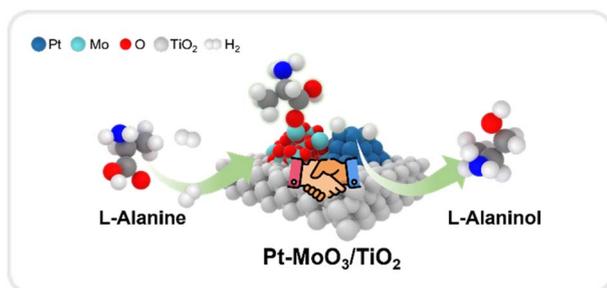
21887



## Carboxylate positional isomerism in metallacycles governs hierarchical assembly pathways

Lingran Liu, Meilin Yu, Wei Tuo, Yue Zhao, Fengmin Zhang and Yan Sun<sup>\*</sup>

21897



## Insights into bifunctional active sites of $\text{Pt-MoO}_3/\text{TiO}_2$ catalysts enabling selective hydrogenation of an amino acid

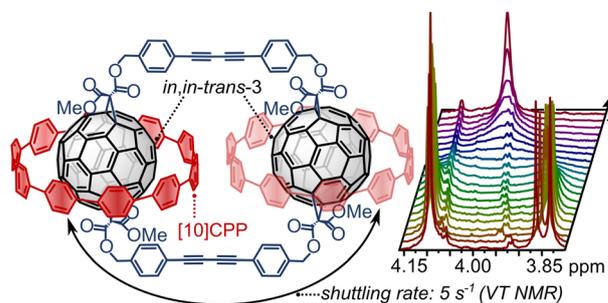
Yundao Jing, Xiaohu Ge, Rui Song, Ningchao Zhu, Jinqian Ming, Nihong An, Yueqiang Cao,<sup>\*</sup> Gang Qian, Xuezhi Duan<sup>\*</sup> and Xinggui Zhou



21908

### Observation of shuttling on the one-second timescale in a [10]cycloparaphenylene/C<sub>60</sub> [2] catenane

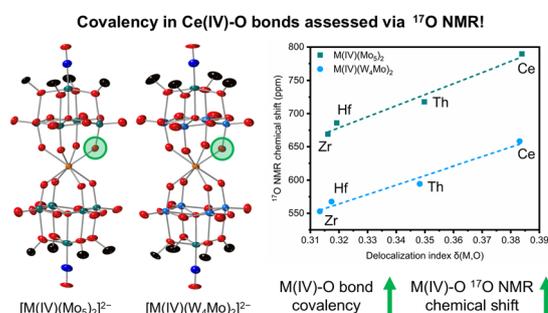
Fabian M. Steudel, Clara Sabrià, Massimo Delle Piane, Ferran Feixas, Xavi Ribas, Giovanni M. Pavan and Max von Delius\*



21917

### Isolation of Ce(IV) centered polyoxoalkoxide sandwich-type complexes allows comparison of metal–oxygen bond covalency

Dominic Shiels,\* Michele Pittalis, Nadeeshan Gunarathna, Adriana C. Berlfein, William W. Brennessel, Michael T. Ruggiero\* and Ellen M. Matson\*



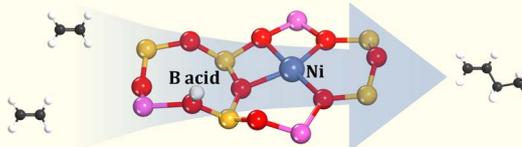
21932

### Brønsted acid-promoted ethylene dimerization to 1-butene over Ni-containing zeolite catalysts

Li Wang, Yuwen Ni, Jingyao Yang, Guangjun Wu, Yuchao Chai\* and Landong Li

☑ TOF = 427954 h<sup>-1</sup>

☑ 1-Butene sel. = 83.6 %



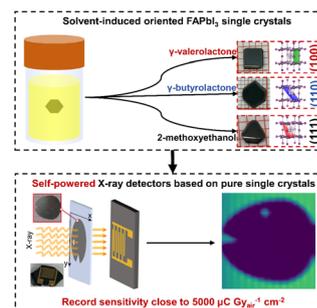
☑ Heterogeneous catalyst

☑ Cocatalyst & solvent free

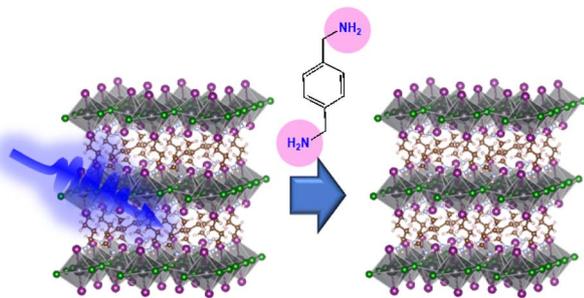
21942

### Solvent-induced orientation of FAPbI<sub>3</sub> single crystals for highly efficient self-powered X-ray detectors

Fang Liu, Yu Zou, Pengxiang Wang, Hu Wang, Jiahao Guo, Yugang Liang, Haifei Wang, Wenji Zhan, Zhengzheng Dang, Jixin Wu, Yanming Wang, Bawei Li, Yanfeng Miao, Yuetian Chen, Yao Wang\* and Yixin Zhao\*



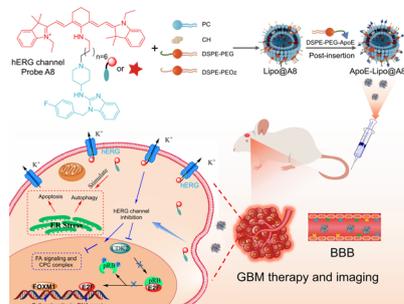
21950



### Design principles of spacer cations for suppressing phase segregation in 2D halide perovskites

Seonhong Min, Manish Mukherjee, Gábor Szabó, Prashant V. Kamat\* and Junsang Cho\*

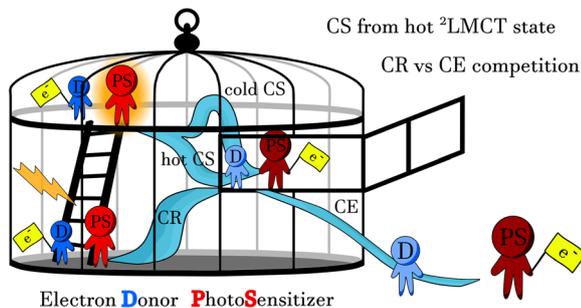
21962



### A novel near-infrared fluorescent hERG potassium channel probe for glioblastoma therapy and imaging

Zhenzhen Liu,\* Li Liu, Tongtong Ban, Xin Wang, Ruihao Li, Xiao Zhang, Yuanwen Wang, Xiaojuan Li, Wei Zhang, Ping Li\* and Bo Tang

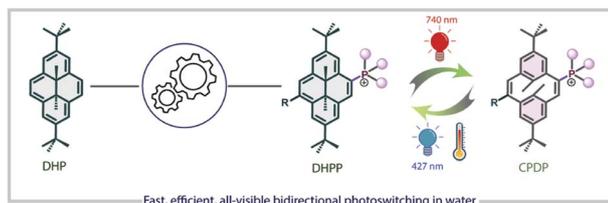
21975



### Captivating bimolecular photoredox dynamics of a ligand-to-metal charge transfer complex

Christina Wegeberg,\* Neus A. Calvet, Mila Krafft, Pavel Chábera, Arkady Yartsev\* and Petter Persson\*

21991



### Installation of cationic phosphorus on dimethyldihydropyrene photoswitches: expanding the atomic repertoire towards far-red photoswitching in water

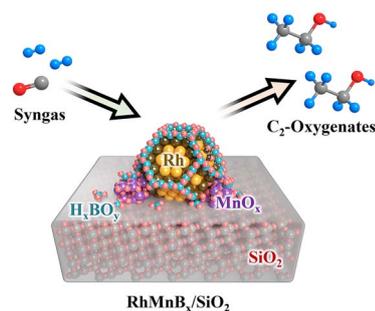
Manik Lal Maity, Sayan Chandra, Samyadeb Mahato and Subhajit Bandyopadhyay\*



22002

### Spontaneous deposition of boron oxide on a rhodium nanostructure for selective conversion of syngas to ethanol

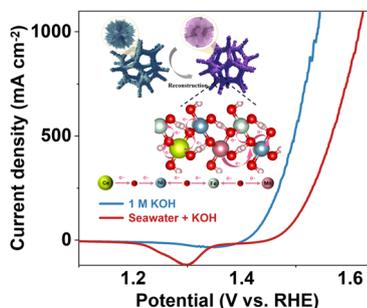
Jiale Xiao, Cao Wang, Haotian Meng, Chengtao Wang,\* Hangjie Li, Yu-Xiao Cheng, Ni Yi, Wentao Yuan, Wei Zhou, Liang Cao,\* Liang Wang and Feng-Shou Xiao\*



22010

### Synergistic spin effects in medium-entropy Ni–Fe–Mn–Ce oxyhydroxides for seawater oxidation

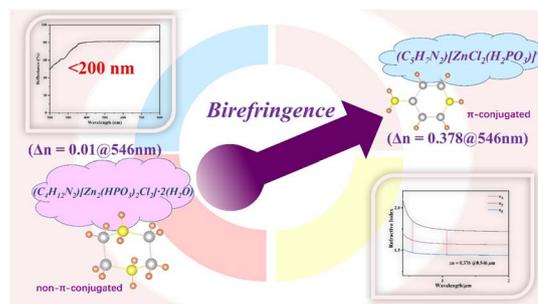
Liyuan Xiao, Xue Bai, Zhenlu Wang and Jingqi Guan\*



22021

### Significant enhancement in the birefringence of metal phosphite halides via the introduction of $\pi$ -conjugated cations

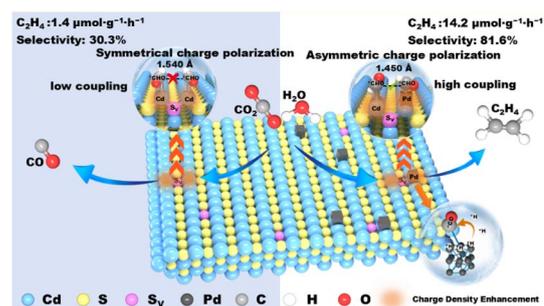
Ru-Ling Tang,\* Yue Wang, Yi-Lei Lv, Bing-Wei Miao, Wenlong Liu and Sheng-Ping Guo\*



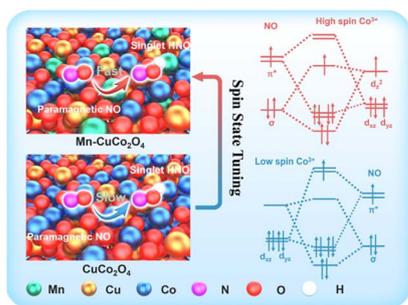
22029

### Engineering Pd-based charge-asymmetrical metal pair sites to promote \*CHO–CHO coupling for selective C<sub>2</sub> photoreduction to C<sub>2</sub>H<sub>4</sub>

Zhijie Pan, Wenbin Liao, Wenbiao Zhang, Qun Liao, Mingyao Zhao, Xionghui Fu, Yuanming Zhang,\* Yi Zhu\* and Qingsheng Gao\*



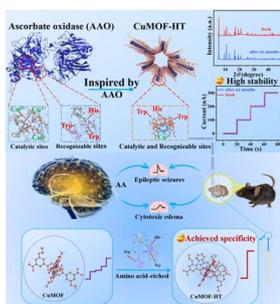
22037



### Manipulating spin-state conversion to promote asymmetric d–p orbital hybridization for high-efficiency nitrate electroreduction to ammonia

Ke Wang, Tong Zhao, Hou Wang, Shiyu Zhang, Rupeng Wang, Meng Wang, Zixiang He, Nan-Qi Ren and Shih-Hsin Ho\*

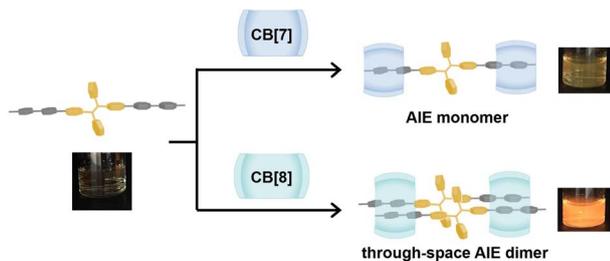
22046



### Enzyme-mimicking metal–organic framework-enabled microsensor for specific electrochemical monitoring *in vivo*

Zhao Yang, Tao Huang,\* Fei Li, Wenbo Huang, Xikui Ouyang, Kangbing Wu and Junxing Hao\*

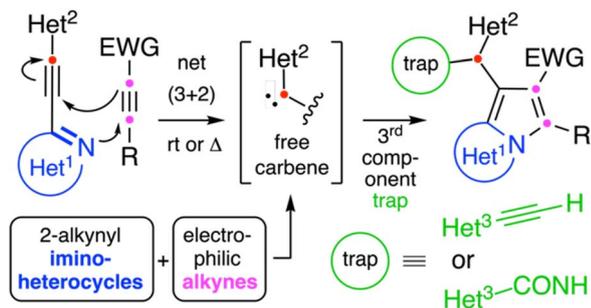
22058



### How many fluorophores are required to achieve AIE?

Tangxin Xiao, Zehuan Huang, Liangliang Zhang, Shuang Jin, Xiaoyi Chen, Hongwei Qian, Guanglu Wu, Jade A. McCune and Oren A. Scherman\*

22065



### 3-Component reactions for accessing heterocycle-rich topologies: trapping of pyrrole-stabilized carbenes via net bimolecular C–H or N–H insertion

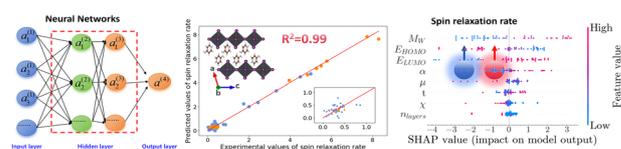
Alexander L. Guzman, Katharine B. Toll and Thomas R. Hoye\*



22071

## Machine learning-driven prediction of ultrafast spin relaxation in metal halide perovskites for spintronic applications

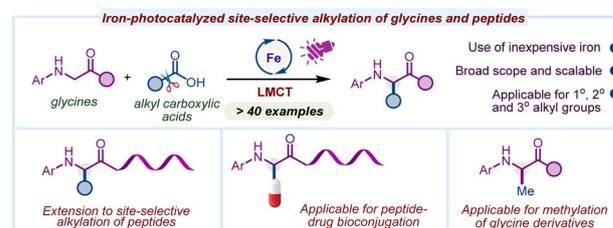
Jianhui Li, Mingxi Chen, Pan Wang, Xiaohong Li, Yuling Huang, Kemi Ding, Lingling Mao, X.-D. Xiang\* and Xihan Chen\*



22084

## Iron photocatalysis towards site-selective C(sp<sup>3</sup>)-H alkylation of glycines and peptides

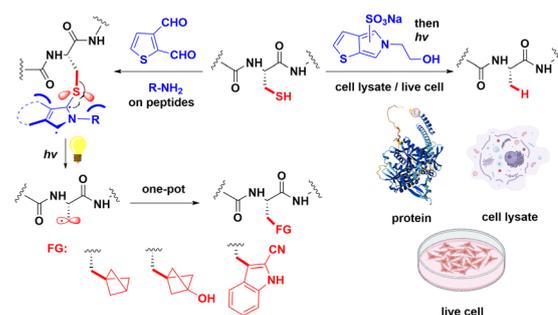
Satya Prakash Panda, M. Siva Prasad, Prahallad Meher, Oliver Reiser\* and Sandip Murarka\*



22091

## Desulfurative modification of cysteine residues in peptides and proteins via the installation and photoexcitation of thieno[2,3-c]-pyrroles

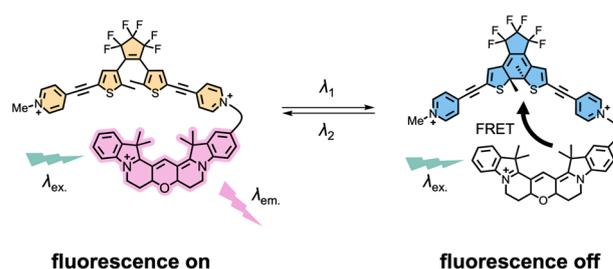
Zijing Chen, Wenjun Wang, Baicheng Chen, Si-Cong Chen, Aimila Aoken, Fanrui Wu, Guihua Zeng and Tuoping Luo\*



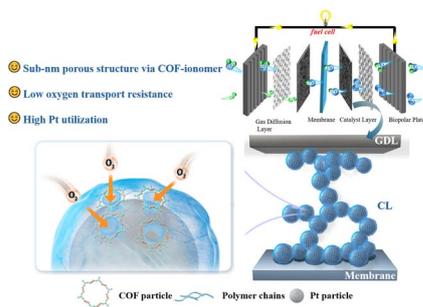
22101

## Design principles for photoswitchable fluorescent dyads

Sili Qiu, Andrew T. Frawley,\* Kathryn G. Leslie, Xingyu Qiu and Harry L. Anderson\*



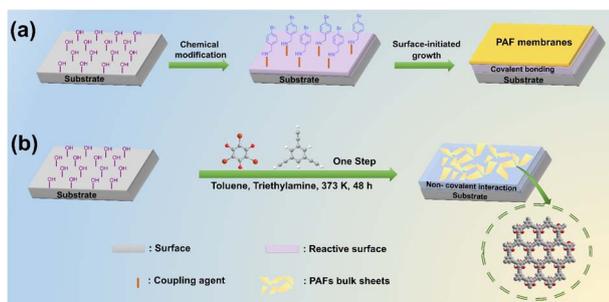
22111



### Achieving ultra-low oxygen transport resistance of fuel cells by microporous covalent organic framework ionomers

Xiaoqin Ma, Xiaoli Lu, Shimei Liang, Caili Yuan, Jingtao Si, Jianchuan Wang\* and Zidong Wei

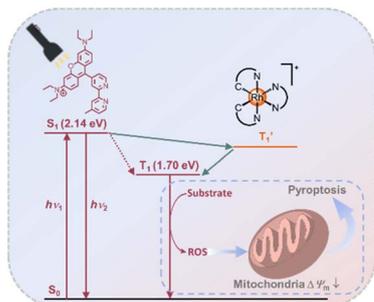
22119



### From surface-assisted synthesis of porous aromatic bulk sheets to readily assembled membranes for nanofiltration

Mengxiao Sun, Geng Tan, Zilong Dou, Jian Song, Xueting Qu, Yuyang Tian\* and Guangshan Zhu\*

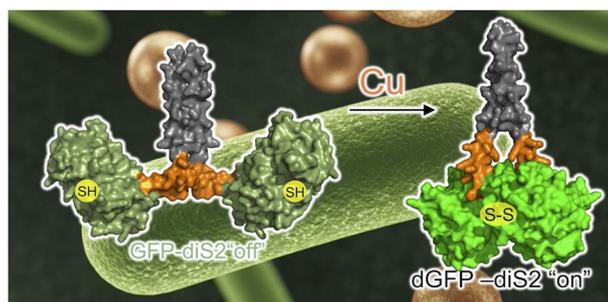
22127



### Rhodamine-functionalised rhodium(III) complexes: dual role as bioimaging agents and controllable reactive oxygen species photosensitisers for photocytotoxicity applications

Katherine Gui-Min Jiang, Fangfang Wei, Peter Kam-Keung Leung, Siye Wu, Kenneth Kam-Wing Lo\* and Keith Man-Chung Wong\*

22136



### Chromophore charge-state switching through copper-dependent homodimerisation of an engineered green fluorescent protein

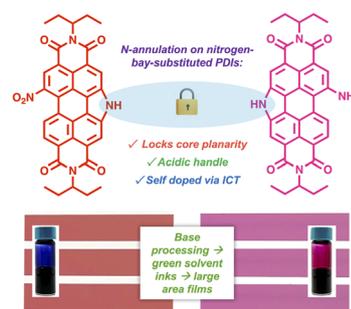
Rochelle D. Ahmed, Danoo Vitsupakorn, Kieran D. Hartwell, Karma Albalawi, Pierre J. Rizkallah, Peter D. Watson and D. Dafydd Jones\*



22147

### Self-doped and planar nitrogen-bay-functionalized perylene diimides: unravelling structure–property relationships

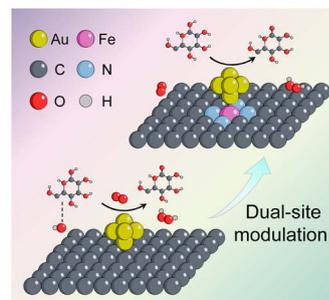
Kathryn M. Wolfe, Zachary T. Gardner, Zachary M. Smith, Alexander Harrison, Chad Risko and Gregory C. Welch\*



22160

### Single atom-bridged Au nanozymes boost glucose oxidase-like activity in acidic media

Xin Luo, Feilong Tan, Zhenglong Mao, Yan Zhang, Yinjun Tang, Canglong Wang, Wenling Gu, Cao Li, Juewen Liu\* and Chengzhou Zhu\*



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### Palladium-catalyzed carbonylative synthesis of acrylamides from alkenyl thianthrenium salts

Ru-Han A, Jiajun Zhang and Xiao-Feng Wu\*

