

# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(32) 12619–13114 (2024)



**Cover**  
See S. Olivia Gunther, Yusen Qiao *et al.*, pp. 12667–12675. Image reproduced by permission of The Regents of the University of California, Lawrence Berkeley National Laboratory from *Chem. Sci.*, 2024, 15, 12667. Cover illustration by Kent Leech for Lawrence Berkeley National Laboratory, Creative Services Office.

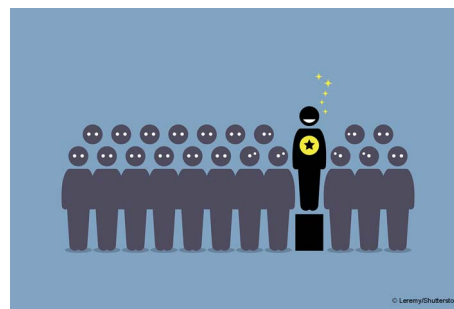


**Inside cover**  
See Masaki Okumura, Tomohide Saio, Takahiro Muraoka *et al.*, pp. 12676–12685. Image reproduced by permission of Takahiro Muraoka from *Chem. Sci.*, 2024, 15, 12676.

## EDITORIAL

12634

Outstanding Reviewers for *Chemical Science* in 2023

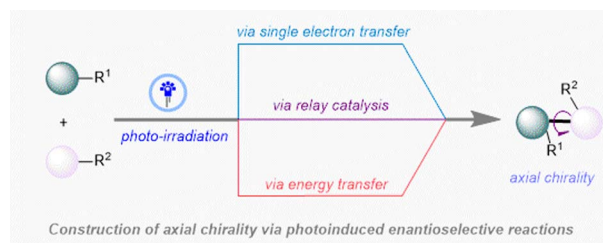


## PERSPECTIVE

12636

Construction of axially chiral molecules enabled by photoinduced enantioselective reactions

Zhaofei Zhang and Lei Dai\*



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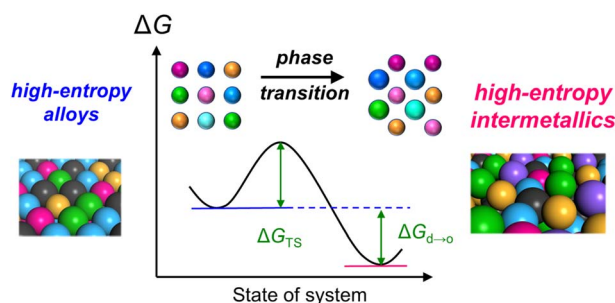
Fundamental questions  
Elemental answers

## REVIEW

12644

**High-entropy intermetallics: emerging inorganic materials for designing high-performance catalysts**

Yuki Nakaya\* and Shinya Furukawa\*

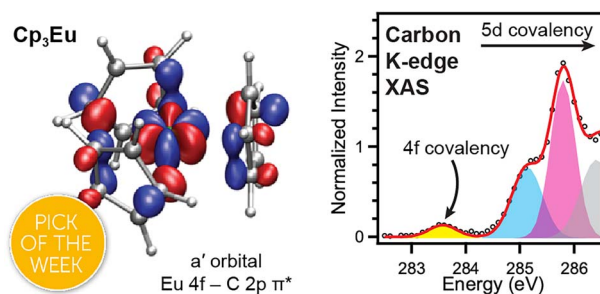


## EDGE ARTICLES

12667

**4f-Orbital mixing increases the magnetic susceptibility of  $Cp_3Eu$** 

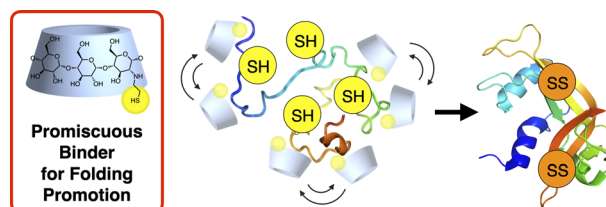
S. Olivia Gunther, Yusen Qiao, Patrick W. Smith, Sierra R. Ciccone, Alexander S. Ditter, Daniel N. Huh, Liane M. Moreau, David K. Shuh, Taoxiang Sun, Polly L. Arnold, Corwin H. Booth, Wibe A. de Jong, William J. Evans, Wayne W. Lukens, Jr and Stefan G. Minasian\*



12676

**Redox-active chemical chaperones exhibiting promiscuous binding promote oxidative protein folding under condensed sub-millimolar conditions**

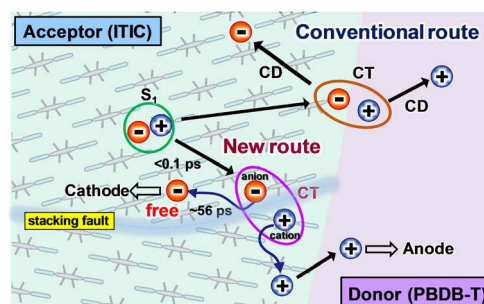
Koki Suzuki, Ryoya Nojiri, Motonori Matsusaki, Takuya Mabuchi, Shingo Kanemura, Kotone Ishii, Hiroyuki Kumeta, Masaki Okumura,\* Tomohide Saio\* and Takahiro Muraoka\*



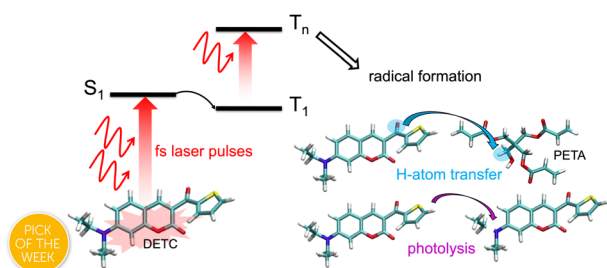
12686

**Boosting charge separation in organic photovoltaics: unveiling dipole moment variations in excited non-fullerene acceptor layers**

Akira Yamakata,\* Kosaku Kato, Takumi Urakami, Sota Tsujimura, Kasumi Murayama, Masahiro Higashi,\* Hirofumi Sato, Yasuhiro Kobori, Tomokazu Umeyama and Hiroshi Imahori\*



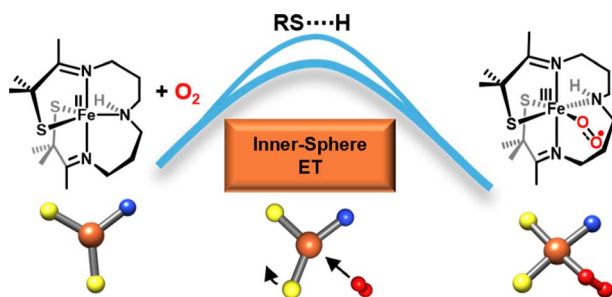
12695



## Two- and three-photon processes during photopolymerization in 3D laser printing

Anna Mauri, Pascal Kiefer, Philipp Neidinger, Tobias Messer, N. Maximilian Bojanowski, Liang Yang, Sarah Walden, Andreas-Neil Unterreiner, Christopher Barner-Kowollik, Martin Wegener, Wolfgang Wenzel and Mariana Kozłowska\*

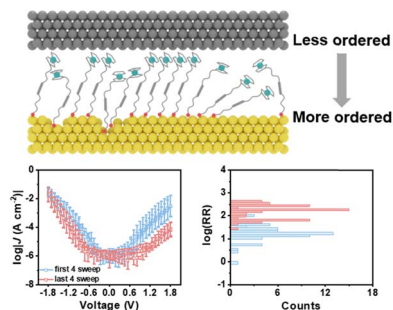
12710



## Exploring the influence of H-bonding and ligand constraints on thiolate ligated non-heme iron mediated dioxygen activation

Maike N. Lundahl, Maria B. Greiner, Marc C. Piquette, Paige M. Gannon, Werner Kaminsky and Julie A. Kovacs\*

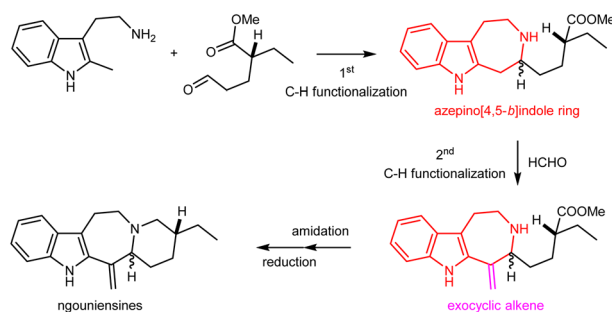
12721



## Dynamically blocking leakage current in molecular tunneling junctions

Yu Xie, Shengzhe Qiu, Qianqian Guo, Chengtai Li, Ningyue Chen, Ziming Zhou, Zhenyu Yang, Zhou Cao, Tao Wang,\* Wei Du,\* Lejia Wang\* and Yuan Li\*

12732



## C–H functionalization of 2-alkyl tryptamines: direct assembly of azepino[4,5-*b*]indoles and total synthesis of ngouniensines

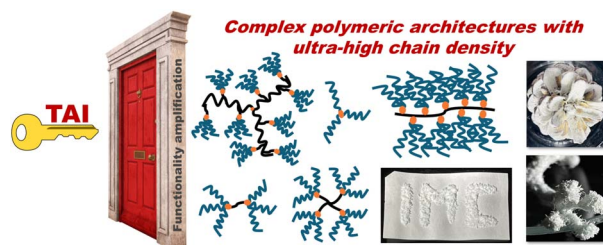
Kejing Xie, Zeyuan Shen, Peng Cheng, Haoxiang Dong, Zhi-Xiang Yu\* and Liansuo Zu\*



12739

## Straightforward synthesis of complex polymeric architectures with ultra-high chain density

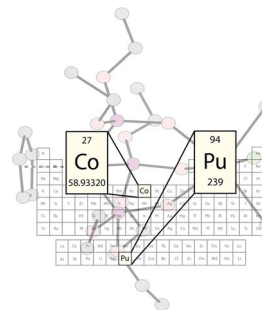
Sachin Gupta, Miroslav Janata, Eva Čadová and Vladimír Raus\*



12754

## $\text{PuCl}_3(\text{CoCp}[\text{OP}(\text{OEt})_2]_3)$ : transuranic elements entering the field of heterometallic molecular chemistry

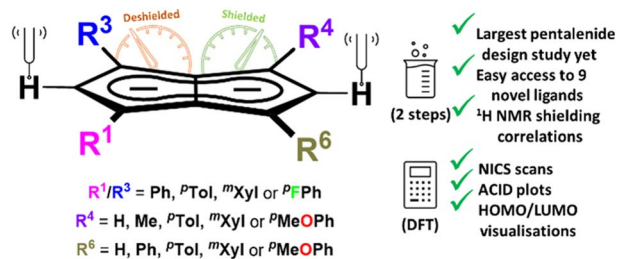
Thomas E. Shaw, Zachary R. Jones, Sara L. Adelman,\* Nickolas H. Anderson, Eric G. Bowes, Eric D. Bauer,\* David Dan, Jan Klouda, Karah E. Knope,\* Stosh A. Kozimor,\* Molly M. MacInnes, Veronika Mocko, Francisca R. Rocha, Harrison D. Root, Benjamin W. Stein, Joe D. Thompson and Jennifer N. Wacker



12765

## Understanding and tuning the electronic structure of pentalenides

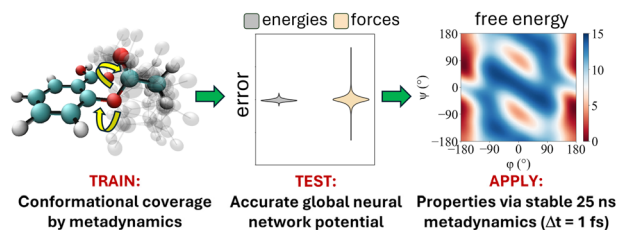
Niko A. Jenek, Andreas Helbig, Stuart M. Boyd, Mandeep Kaur, Hugh J. Sanderson, Shaun B. Reeksting, Gabriele Kociok-Köhn, Holger Helten\* and Ulrich Hintermair\*



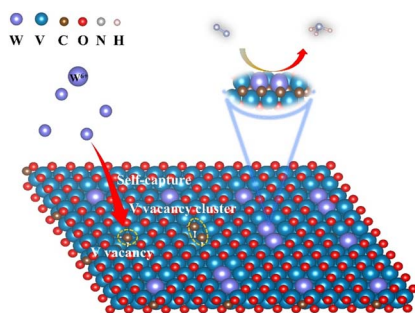
12780

## Stable and accurate atomistic simulations of flexible molecules using conformationally generalisable machine learned potentials

Christopher D. Williams,\* Jas Kalayan, Neil A. Burton and Richard A. Bryce\*



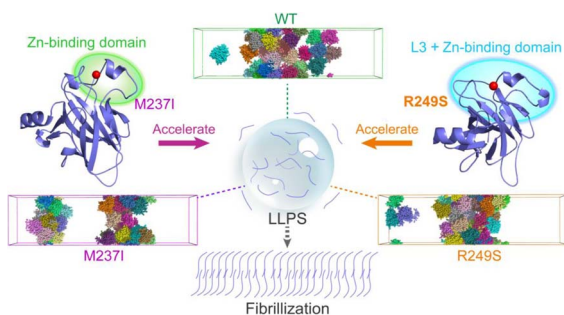
12796



### Efficient N<sub>2</sub> electroreduction enabled by linear charge transfer over atomically dispersed W sites

Jin Wan, Dong Liu, Chuanzhen Feng, Huijuan Zhang\* and Yu Wang\*

12806

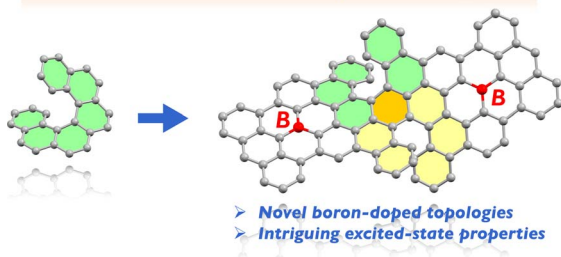


### Multiscale simulations reveal the driving forces of p53C phase separation accelerated by oncogenic mutations

Yawei Yu, Qian Liu, Jiyuan Zeng, Yuan Tan, Yiming Tang and Guanghong Wei\*

12819

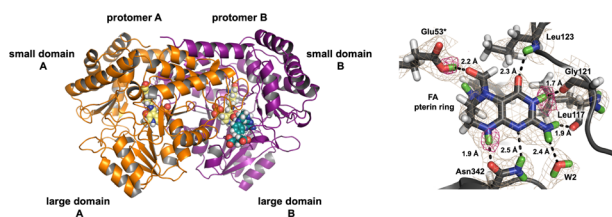
### From Helicene to Boron-Doped Carbohelicene



### Boron-doped double [6]carbohelicenes: a combination of helicene and boron-doped $\pi$ -systems

Yujia Liu, Liuzhong Yuan, Zengming Fan, Jingyuan Yang, Yue Wang and Chuandong Dou\*

12827



### Universality of critical active site glutamate as an acid–base catalyst in serine hydroxymethyltransferase function

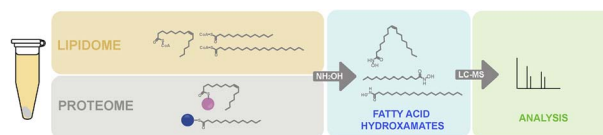
Victoria N. Drago, Robert S. Phillips and Andrey Kovalevsky\*



12845

## Quantitative analysis of protein lipidation and acyl-CoAs reveals substrate preferences of the S-acylation machinery

Carla Busquets-Hernández, Silvia Ribó, Esther Gratacós-Batlle, Daniel Carbajo, Alexandra Tsitsia, Juan B. Blanco-Canosa, Luke H. Chamberlain and Gemma Triola\*



12856

## Asymmetric total syntheses of sarglamides A, C, D, E, and F

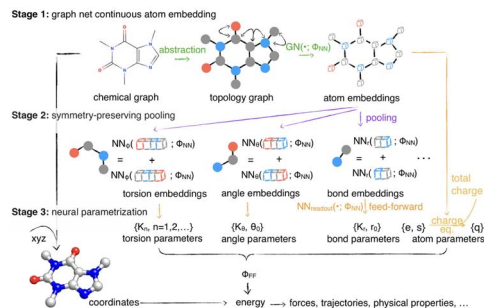
Ryungwoo Kim, Yanting Wu and Rongbiao Tong\*



12861

## Machine-learned molecular mechanics force fields from large-scale quantum chemical data

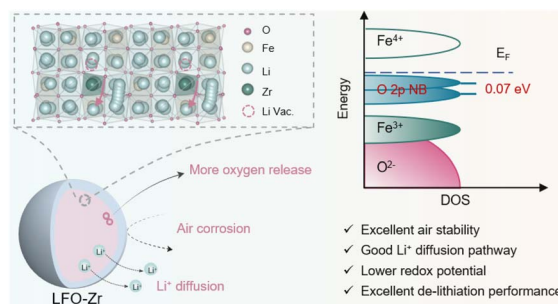
Kenichiro Takaba,\* Anika J. Friedman, Chapin E. Cavender, Pavan Kumar Behara, Iván Pulido, Michael M. Henry, Hugo MacDermott-Opeskin, Christopher R. Iacovella, Arnav M. Nagle, Alexander Matthew Payne, Michael R. Shirts, David L. Mobley, John D. Chodera\* and Yuanqing Wang\*



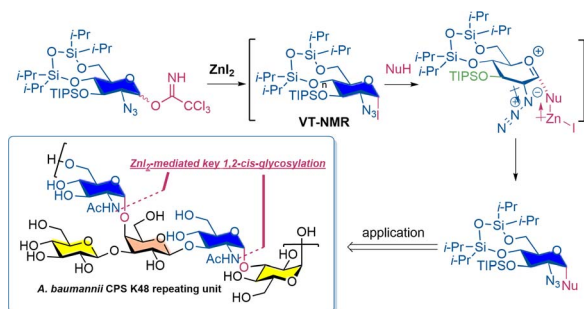
12879

## Defect engineering of air-stable $\text{Li}_5\text{FeO}_4$ towards an ultra-high capacity cathode prelithiation additive

Bin Zhu, Naifeng Wen, Jingyang Wang,\* Qiyu Wang, Jingqiang Zheng and Zhian Zhang\*



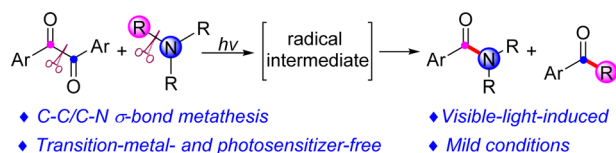
12889



### Zinc(II)-mediated stereoselective construction of 1,2-cis 2-azido-2-deoxy glycosidic linkage: assembly of *Acinetobacter baumannii* K48 capsular pentasaccharide derivative

Xiaoya Zhao, Han Ding, Aoxin Guo, Xuemei Zhong, Siai Zhou, Guoqing Wang, Yuhua Liu, Akihiro Ishiwata,\* Katsunori Tanaka, Hui Cai,\* Xue-Wei Liu\* and Feiqing Ding\*

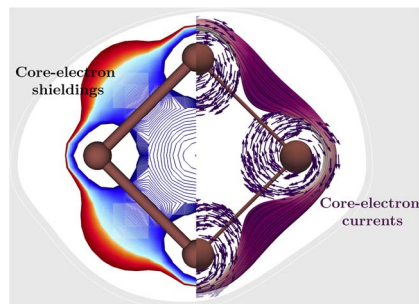
12900



### Intermolecular C-C/C-N $\sigma$ -bond metathesis enabled by visible light

Rujuan Li, Renqin Zhan, Yatao Lang, Chao-Jun Li\* and Huiying Zeng\*

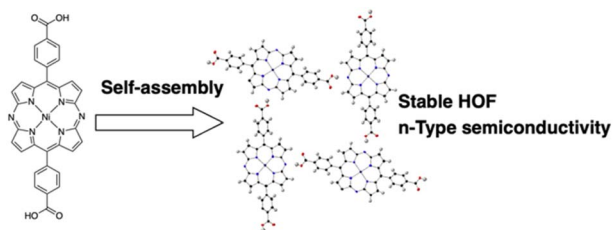
12906



### Core-electron contributions to the magnetic response of molecules with heavy elements and their significance in aromaticity assessments

Mesías Orozco-Ic,\* Luis Soriano-Agueda, Dage Sundholm, Eduard Matito\* and Gabriel Merino\*

12922



### An n-type semiconducting diazaporphyrin-based hydrogen-bonded organic framework

Takahiro Sakurai, Tappei Tanabe, Hiroaki Iguchi, Zhuowei Li, Wakana Matsuda, Yusuke Tsutsui, Shu Seki,\* Ryotaro Matsuda\* and Hiroshi Shinokubo\*

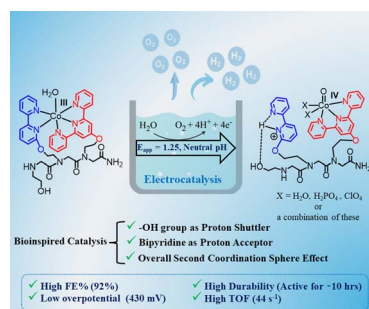




12928

## An intramolecular cobalt-peptoid complex as an efficient electrocatalyst for water oxidation at low overpotential

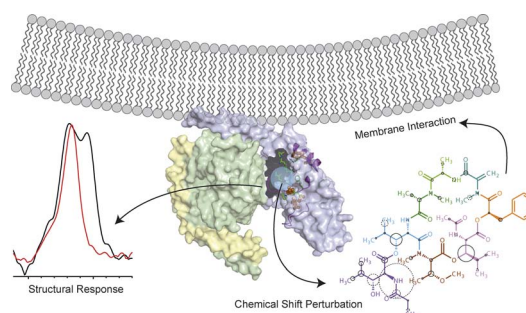
Suraj Pahar and Galia Maayan\*



12939

## Structural response of G protein binding to the cyclodepsipeptide inhibitor FR900359 probed by NMR spectroscopy

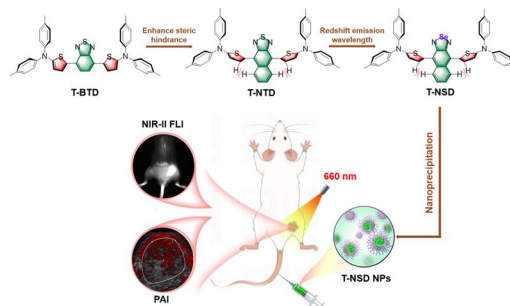
Christian Bonifer, Wiebke Hanke, Jonas Mühle, Frank Löh, Johanna Becker-Baldus, Jessica Nagel, Gebhard F. X. Schertler, Christa E. Müller, Gabriele M. König, Daniel Hilger\* and Clemens Glaubitz\*



12957

## Structural modulation of aggregation-induced emission luminogens for NIR-II fluorescence imaging/photoacoustic imaging of tumors

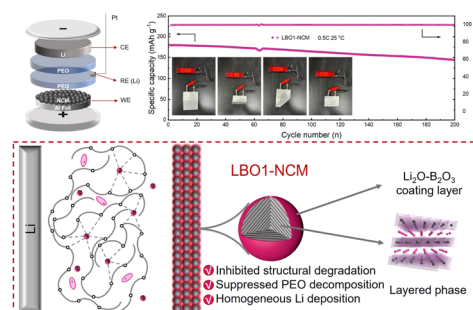
Xue Liu, Yonghong Tan, Jianyu Zhang, Weigeng Huang, Dingyuan Yan,\* Dong Wang\* and Ben Zhong Tang\*



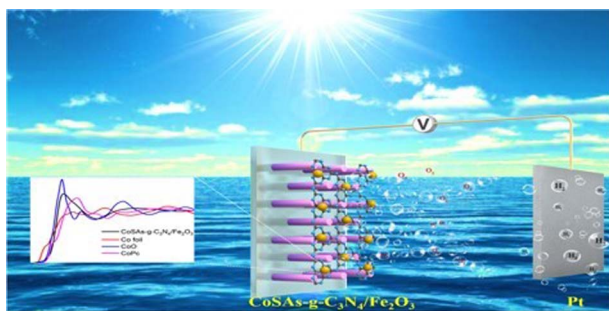
12964

## Improving the interfacial stability of ultrahigh-nickel cathodes with PEO-based electrolytes by targeted chemical reactions

Yuqing Dai, Zihan Hou, Gui Luo, Duo Deng, Wenjie Peng, Zhixing Wang, Huajun Guo, Xinhai Li, Guochun Yan, Hui Duan, Wenchao Zhang and Jiexi Wang\*



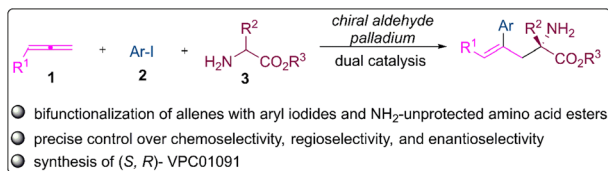
12973



### Enhanced photoelectrochemical water splitting performance of $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoanodes through Co-modification with Co single atoms and g-C<sub>3</sub>N<sub>4</sub>

Juan Wu, Xiaodi Du, Mingjie Li, Hongyu Chen, Bin Hu, Hongwei Ding, Nannan Wang, Lin Jin\* and Weisheng Liu\*

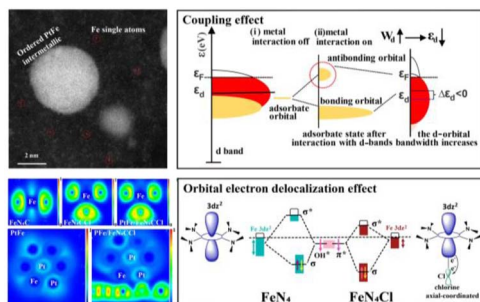
12983



### Asymmetric bifunctionalization of allenes with aryl iodides and amino acids enabled by chiral aldehyde/palladium combined catalysis

Hao Zhang, Wei Wen,\* Yu-Yang Wang, Ze-Xi Lu, Jin-Long Liu, Zhu-Lian Wu, Tian Cai and Qi-Xiang Guo\*

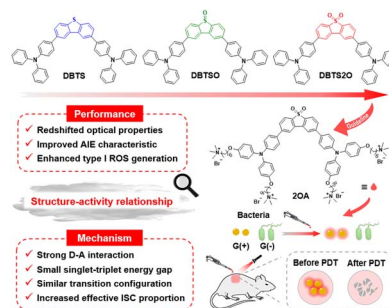
12989



### Orbital electron delocalization of axial-coordinated modified FeN<sub>4</sub> and structurally ordered PtFe intermetallic synergistically for efficient oxygen reduction reaction catalysis

Chenzhong Wu, Meida Chen, Bin Wang, Leqing Luo, Qian Zhou, Guangtao Mao, Yuan Xiong and Qingmei Wang\*

13001



### Sulfur oxidation states manipulate excited state electronic configurations for constructing highly efficient organic type I photosensitizers

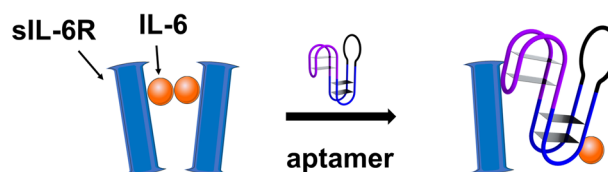
Jianye Gong, Xiaopeng Wang, Weijing Zhang, Yifan Wu, Kai Li, Renmanduhu Sha, Lingxiu Liu, Chunbin Li, Lina Feng, Guoyu Jiang, Jianguo Wang\* and Ben Zhong Tang



13011

### Evolution of a bispecific G-quadruplex-forming circular aptamer to block IL-6/sIL-6R interaction for inflammation inhibition

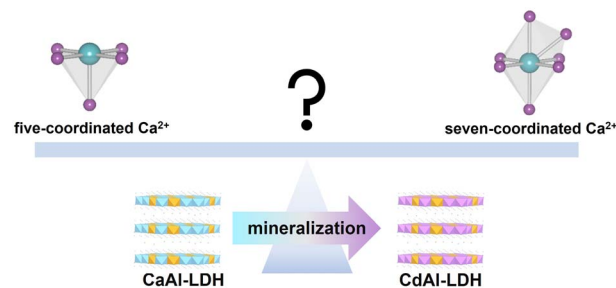
Lili Yao, Lei Wang, Shuai Liu, Hao Qu, Yu Mao,\* Yingfu Li\* and Lei Zheng\*



13021

### Theory-driven design of cadmium mineralizing layered double hydroxides for environmental remediation

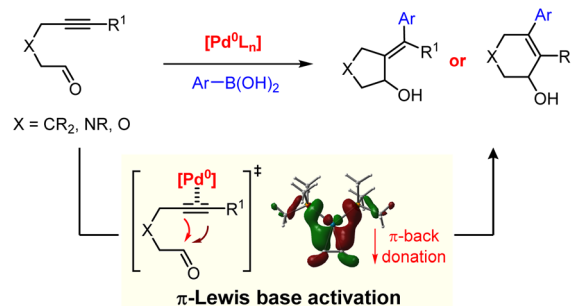
Zixian Li, Nuo Xu, Jing Ren, Haigang Hao, Rui Gao, Xiangui Kong, Hong Yan, Xiao Hua, Yung-Kang Peng, Shulan Ma, Dermot O'Hare and Yufei Zhao\*



13032

### Metal $\pi$ -Lewis base activation in palladium(0)-catalyzed *trans*-alkylative cyclization of alkynals

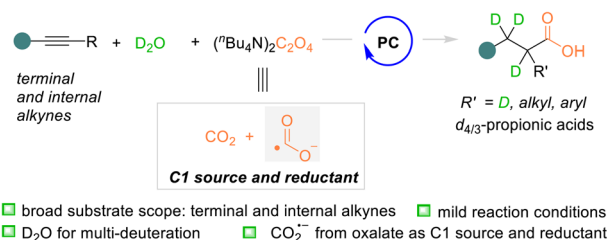
Lei Zhu, Bo Zhao, Ke Xie, Wu-Tao Gui, Sheng-Li Niu, Peng-Fei Zheng, Ying-chun Chen, Xiao-Wei Qi\* and Qin Ouyang\*



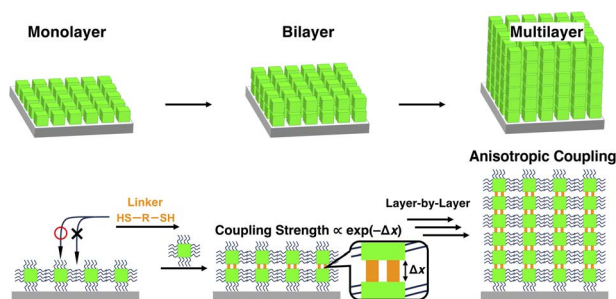
13041

### Photocatalytic deutero-carboxylation of alkynes with oxalate

Pei Xu, Hao-Qiang Jiang, Hui Xu, Sai Wang, Hui-Xian Jiang, Song-Lei Zhu, Long Yin,\* Dong Guo\* and Xu Zhu\*



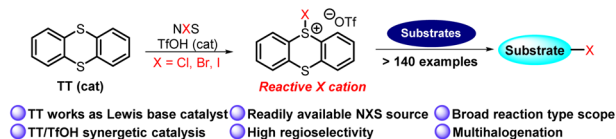
13049



### Anisotropic electronic coupling in three-dimensional assembly of CsPbBr<sub>3</sub> quantum dots

Kazushi Enomoto,\* Retno Miranti, Jianjun Liu, Rinkei Okano, Daishi Inoue, DaeGwi Kim\* and Yong-Jin Pu\*

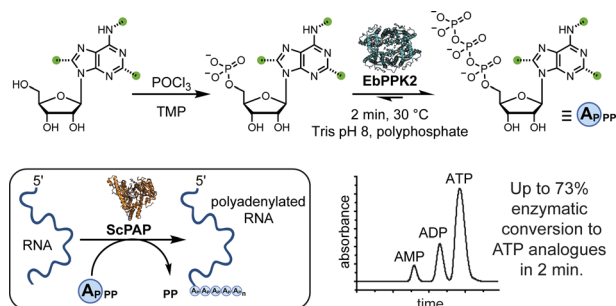
13058



### Thianthrene/TfOH-catalyzed electrophilic halogenations using *N*-halosuccinimides as the halogen source

Haofeng Shi, Jingran Zhang, Xuemin Li, Jiabin He, Yuli Sun, Jialiang Wu and Yunfei Du\*

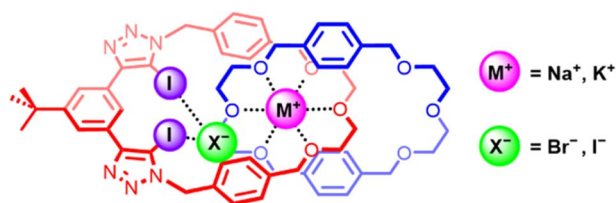
13068



### Chemo-enzymatic production of base-modified ATP analogues for polyadenylation of RNA

Rachel M. Mitton-Fry,\* Jannik Eschenbach, Helena Schepers, René Rasche, Mehmet Erguven, Daniel Kümmel, Andrea Rentmeister\* and Nicolas V. Cornelissen\*

13074



### Selective ion-pair binding and extraction: NaX > KX

### Selective sodium halide over potassium halide binding and extraction by a heteroditopic halogen bonding [2]catenane

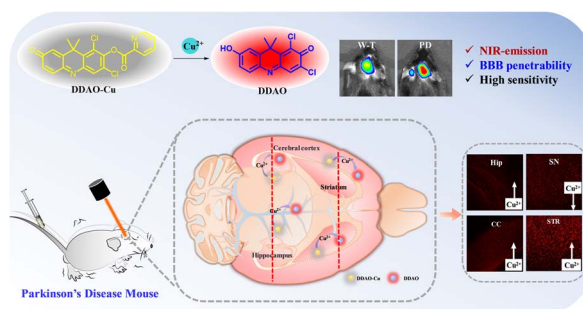
Hui Min Tay, Andrew Docker, Carol Hua and Paul D. Beer\*



13082

### A novel NIR fluorescent probe for copper(II) imaging in Parkinson's disease mouse brain

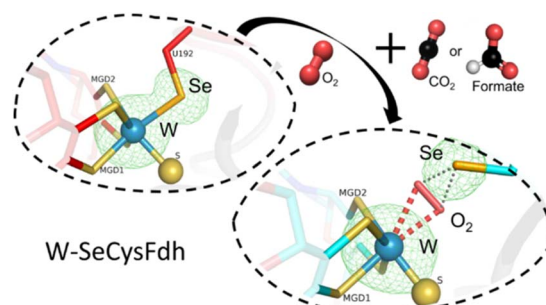
Jianmei Chen, Rongqing Luo, Shuang Li, Jinping Shao, Ting Wang, Shumei Xie, Li Xu,\* Qiuyun You,\* Shumin Feng\* and Guoqiang Feng\*



13090

### Substrate-dependent oxidative inactivation of a W-dependent formate dehydrogenase involving selenocysteine displacement

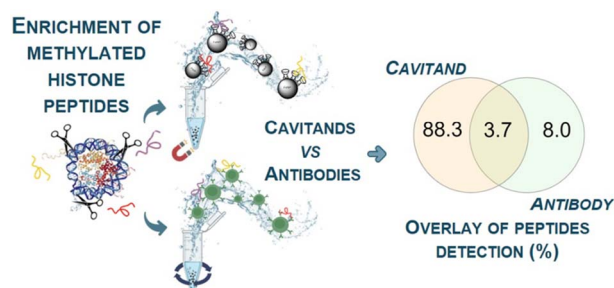
Guilherme Vilela-Alves, Rita R. Manuel, Aldino Viegas, Philippe Carpentier, Frédéric Biaso, Bruno Guigliarelli, Inês A. C. Pereira,\* Maria João Romão\* and Cristiano Mota\*



13102

### Enrichment of histone tail methylated lysine residues via cavitand-decorated magnetic nanoparticles for ultra-sensitive proteomics

Martina Orlandini, Alex Bonacini, Alessia Favero, Andrea Secchi, Laura Lazzarini, Roberto Verucchi, Enrico Dalcanale, Alessandro Pedrini, Simone Sidoli\* and Roberta Pinalli\*



13111

### Correction: Asymmetric catalytic [1,3]- or [3,3]-sigmatropic rearrangement of 3-allyloxy-4H-chromenones and their analogues

Yi Li, Lichao Ning, Qi Tang, Kexin Lan, Bingqian Yang, Qianchi Lin, Xiaoming Feng\* and Xiaohua Liu\*

