

# Chemical Science

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## IN THIS ISSUE

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See Xiaoyu Wu and Jianwen Jiang, pp. 16467–16479. Image reproduced by permission of Xiaoyu Wu and Jianwen Jiang from *Chem. Sci.*, 2024, **15**, 16467.



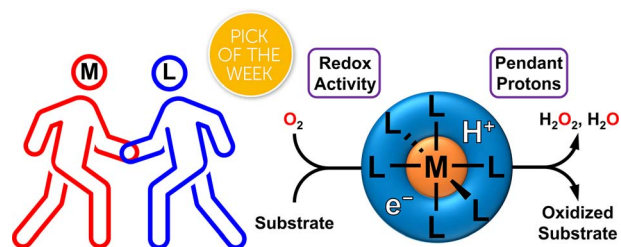
**Inside cover**  
See Paola Posocco, Volodymyr Sashuk *et al.*, pp. 16480–16484. Image reproduced by permission of Volodymyr Sashuk from *Chem. Sci.*, 2024, **15**, 16480. Artwork created by Sofiya Sashuk.

## PERSPECTIVES

16409

### Leveraging ligand-based proton and electron transfer for aerobic reactivity and catalysis

Kate A. Jesse\* and John S. Anderson\*

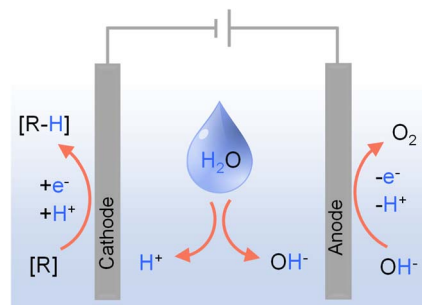


Leveraging **Metal-ligand Cooperativity** for O<sub>2</sub> Utilization

16424

### Electricity-driven organic hydrogenation using water as the hydrogen source

Bidyut Kumar Kundu and Yujie Sun\*





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## REVIEW

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## Flexible piezoelectric materials and strain sensors for wearable electronics and artificial intelligence applications

Yanyu Chen, Xiaohong Zhang and Chao Lu\*



## EDGE ARTICLES

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## Precision-engineered metal–organic frameworks: fine-tuning reverse topological structure prediction and design

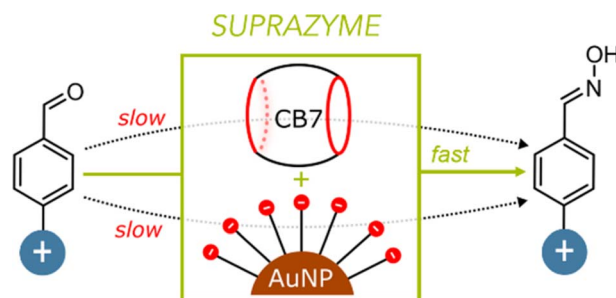
Xiaoyu Wu and Jianwen Jiang\*



16480

## Creating a suprazyme: integrating a molecular enzyme mimic with a nanozyme for enhanced catalysis

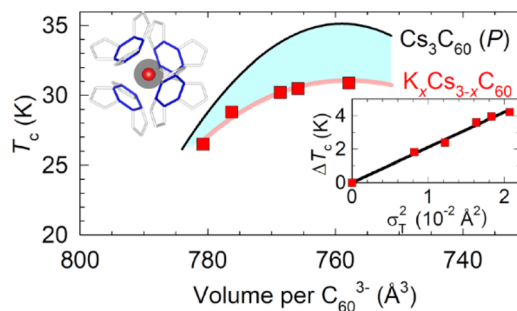
Pavlo Hyziuk, Matteo Flaibani, Paola Posocco\* and Volodymyr Sashuk\*



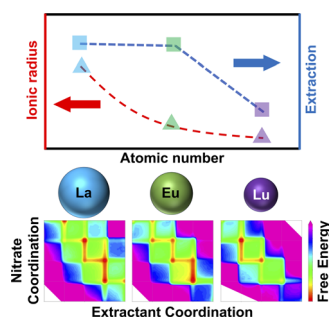
16485

## Fulleride superconductivity tuned by elastic strain due to cation compositional disorder

H. Esmā Okur, Ross H. Colman, Yasuhiro Takabayashi, Peter Jeglič, Yasuo Ohishi, Kenichi Kato, Denis Arčon, Yoshiki Kubota and Kosmas Prassides\*



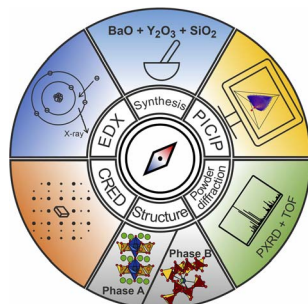
16494



### Metadynamics investigation of lanthanide solvation free energy landscapes and insights into separations energetics

Xiaoyu Wang,\* Allison A. Peroutka, Dmytro V. Kravchuk, Jenifer C. Shafer, Richard E. Wilson and Michael J. Servis\*

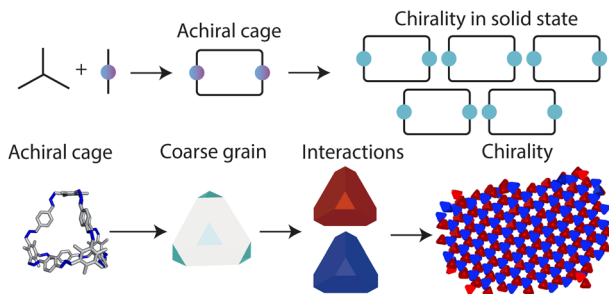
16503



### Navigation through high-dimensional chemical space: discovery of $Ba_5Y_{13}[SiO_4]_8O_{8.5}$ and $Ba_3Y_2[Si_2O_7]_2$

Nataliya L. Gulay, Marco Zanella, Craig M. Robertson, Daniel Ritchie, Manel Sonni, Matthew A. Wright, Jon A. Newnham, Cara J. Hawkins, Jayne Whitworth, Bhupendra P. Mali, Hongjun Niu, Matthew S. Dyer, Christopher M. Collins, Luke M. Daniels, John B. Claridge and Matthew J. Rosseinsky\*

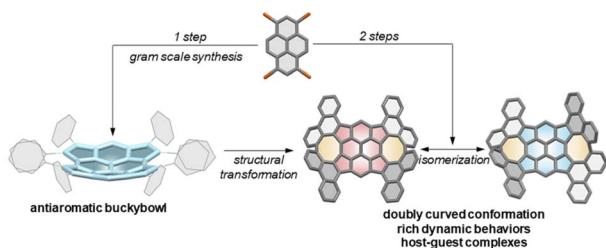
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### Introducing chirality in porous organic cages through solid-state interactions

Emma H. Wolpert\* and Kim E. Jelfs\*

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### $\pi$ -extended pyrenes: from an antiaromatic buckybowl to doubly curved nanocarbons with gulf architectures

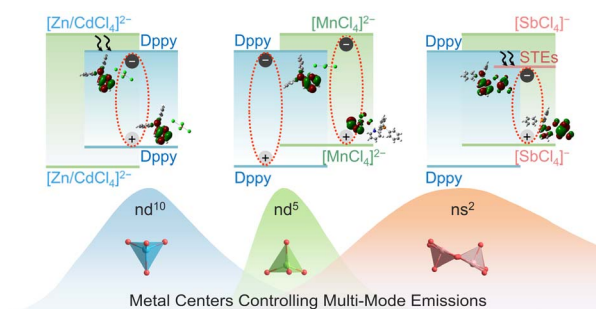
Binbin Liu, Zhengxiong Jin, Xinyue Liu, Lanfei Sun, Cao Yang\* and Lei Zhang\*



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### Optical activity levels of metal centers controlling multi-mode emissions in low-dimensional hybrid metal halides for anti-counterfeiting and information encryption

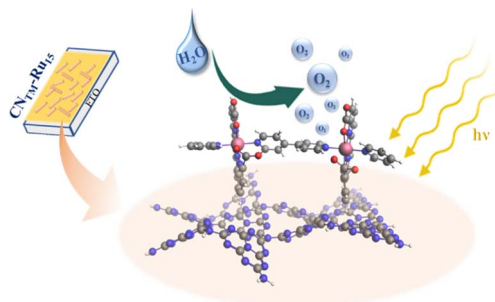
Qiqiong Ren, Guojun Zhou,\* Yilin Mao, Nan Zhang, Jian Zhang and Xian-Ming Zhang\*



16546

### Supramolecular interaction of a molecular catalyst with a polymeric carbon nitride photoanode enhances photoelectrochemical activity and stability at neutral pH

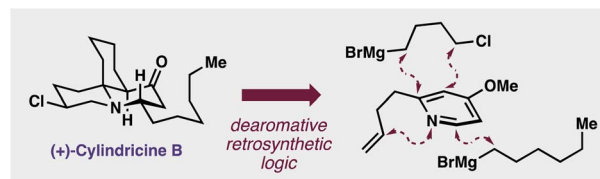
Sanjit Mondal, Martina Salati, Marco Nicaso, Josep Albero, Mireia Segado-Centellas, Michael Volokh, Carles Bo,\* Hermenegildo Garcia, Marcos Gil-Sepulcre,\* Antoni Llobet\* and Menny Shalom\*



16554

### Enantioselective total synthesis of (+)-cylindricine B

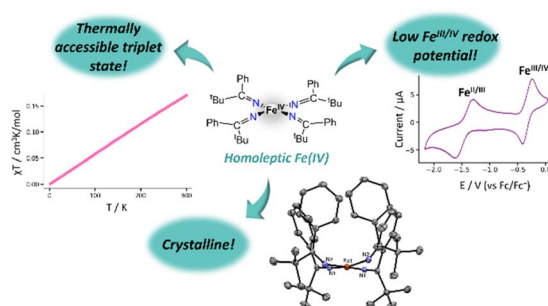
Dallas M. Dukes, Victor K. Atanassov and Joel M. Smith\*



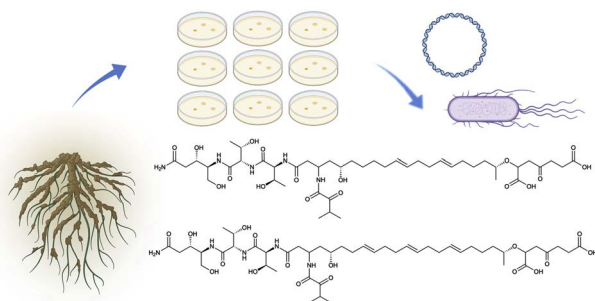
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### A homoleptic Fe(IV) ketimide complex with a low-lying excited state

Phoebe R. Hertler, Arturo Sauza-de la Vega, Andrea Darù, Arup Sarkar, Richard A. Lewis, Guang Wu, Laura Gagliardi\* and Trevor W. Hayton\*



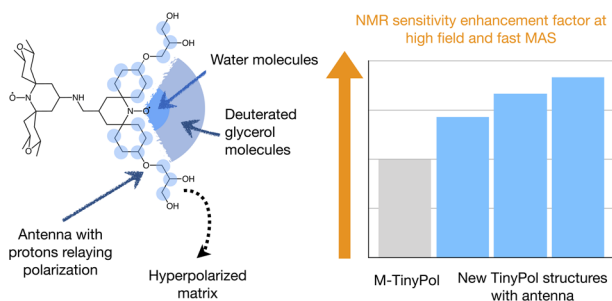
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### Discovery of megapolipeptins by genome mining of a *Burkholderiales* bacteria collection

Bruno S. Paulo, Michael J. J. Recchia, Sanghoon Lee, Claire H. Fergusson, Sean B. Romanowski, Antonio Hernandez, Nyssa Krull, Dennis Y. Liu, Hannah Cavanagh, Allyson Bos, Christopher A. Gray, Brian T. Murphy, Roger G. Linington\* and Alessandra S. Eustaquio\*

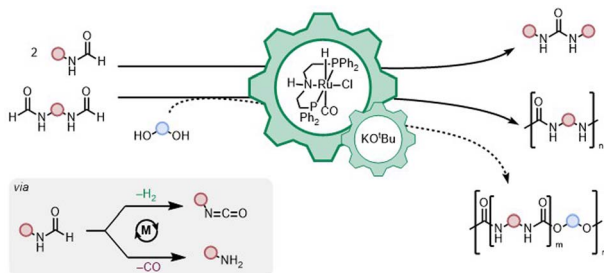
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### Efficient DNP at high fields and fast MAS with antenna-sensitized dinitroxides

Lorenzo Niccoli, Gilles Casano, Georges Menzildjian, Maxim Yulikov, Thomas Robinson, Salah-Eddine Akrial, Zhuoran Wang, Christian Reiter, Armin Porea, Didier Siri, Amrit Venkatesh, Lyndon Emsley, David Gajan, Moreno Lelli,\* Olivier Ouari\* and Anne Lesage\*

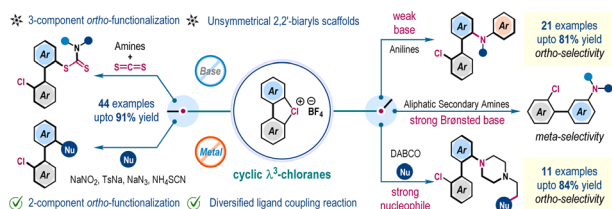
16594



### Exploiting decarbonylation and dehydrogenation of formamides for the synthesis of ureas, polyureas, and poly(urea-urethanes)

James Luk, Alister S. Goodfellow, Nachiket Deepak More, Michael Bühl\* and Amit Kumar\*

16605



### Metal-free site-selective functionalization with cyclic diaryl $\lambda^3$ -chloranes: suppression of benzyne formation for ligand-coupling reactions

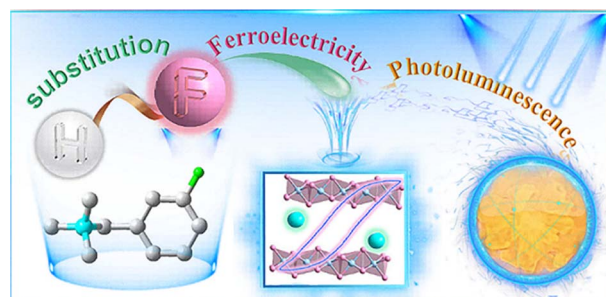
Koushik Patra, Manas Pratim Dey and Mahiuddin Baidya\*



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## The H/F substitution strategy can achieve large spontaneous polarization in 1D hybrid perovskite ferroelectrics

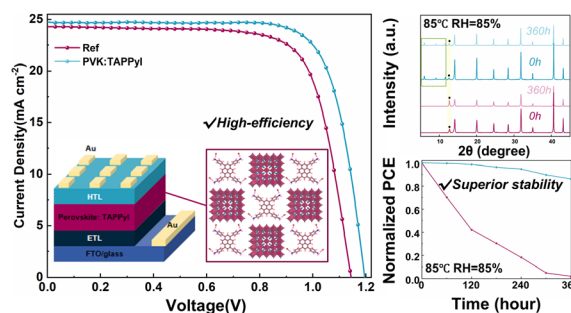
Jiu-Yang Liu, Meng-Meng Lun, Zhi-Jie Wang, Jun-Yi Li, Kun Ding, Da-Wei Fu,\* Hai-Feng Lu\* and Yi Zhang\*



16618

## Incorporation of 2D pyreneammonium iodide for enhancing the efficiency and stability of perovskite solar cells

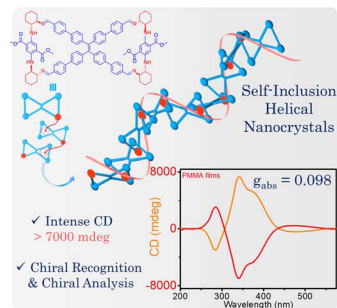
Zhongquan Wan,\* Yuanxi Wang, Hui Lu, Runmin Wei, Haomiao Yin, Huaibiao Zeng, Muhammad Azam, Junsheng Luo\* and Chunyang Jia\*



16627

## Highly enhanced chiroptical effect from self-inclusion helical nanocrystals of tetraphenylethylene bimarocycles

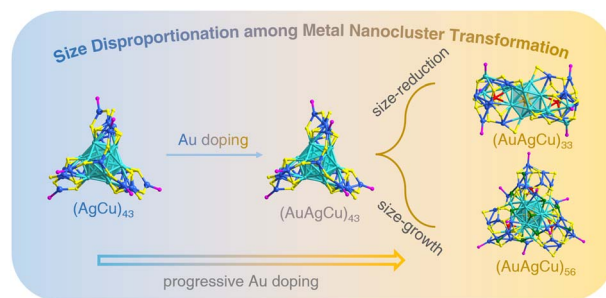
Ming Hu, Feng-Ying Ye, Wei Yu, Kang Sheng, Zhi-Rong Xu, Jin-Jin Fu, Xin Wen, Hai-Tao Feng,\* Minghua Liu and Yan-Song Zheng\*



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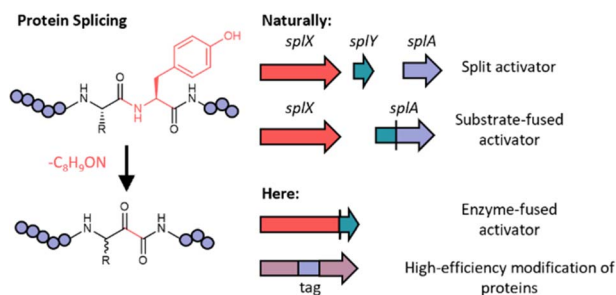
## Size disproportionation among nanocluster transformations

Chen Zhu, Luyao Lu, Fei Li, Xi Kang\* and Manzhou Zhu





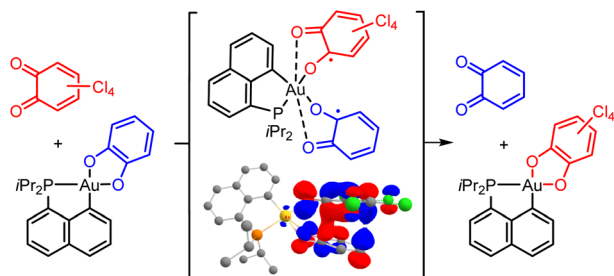
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### A structurally conserved helix enables leader-independent tyramine splicing of proteins

Daniel Richter, Alicia Courvoisier-Clément, Anna Lisa Vagstad, Sarolt Magyari and Jörn Piel\*

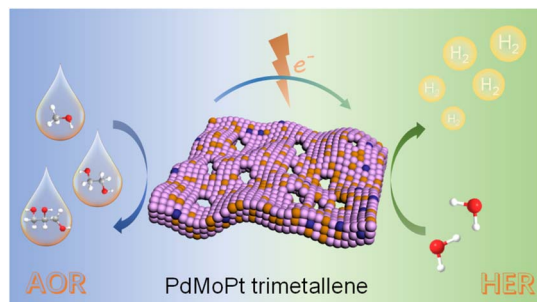
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### Catechol/*o*-benzoquinone exchange at gold(III)

Félix León, Yago García-Rodeja, Sonia Mallet-Ladeira, Karinne Miqueu,\* György Szalóki\* and Didier Bourissou\*

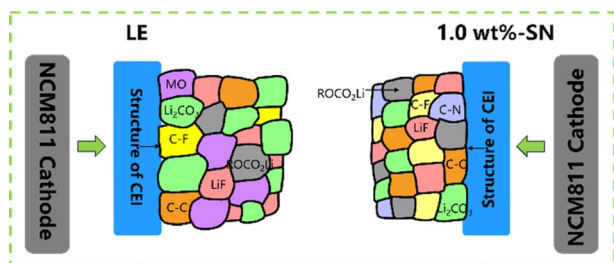
16660



### Bifunctional PdMoPt trimetallic alloy boosts alcohol-water electrolysis

Junfeng Liu,\* Tong Li, Qiuxia Wang, Haiting Liu, Jingjing Wu, Yanping Sui, Huaming Li, Pengyi Tang\* and Yong Wang\*

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### Simultaneous modulation of cathode/anode and electrolyte interfaces via a nitrile additive for high-energy-density lithium-metal batteries

Ziye Wang, Yingshuai Wang, Yuhang Xin, Qingbo Zhou, Xiangyu Ding, Lei Liu, Tinglu Song, Feng Wu, Zhongbao Wei\* and Hongcai Gao\*

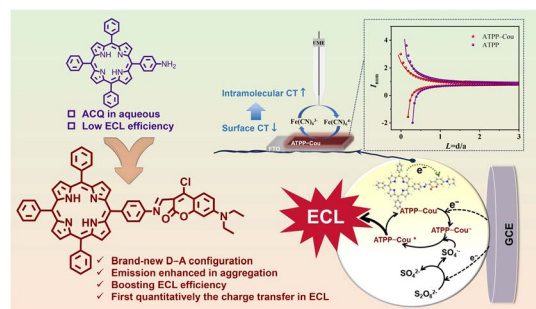




16681

### Insight into the charge transfer behavior of an electrochemiluminescence sensor based on porphyrin–coumarin derivatives with a donor–acceptor configuration

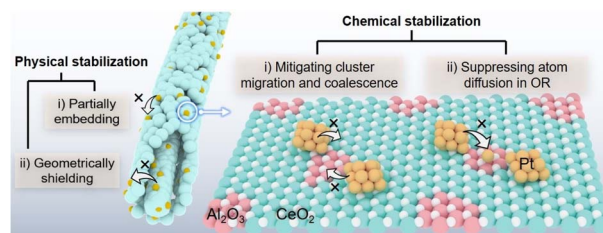
Hui Xiao, Yali Wang, Yaqi Zhao, Rongfang Zhang, Kainan Kang, Yanjun Feng, Yuling Gao, Huixia Guo, Bingzhang Lu,<sup>\*</sup> Peiyao Du<sup>\*</sup> and Xiaoquan Lu<sup>\*</sup>



16688

### Stabilizing ultra-close Pt clusters on all-in-one CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> fibril-in-tubes against sintering

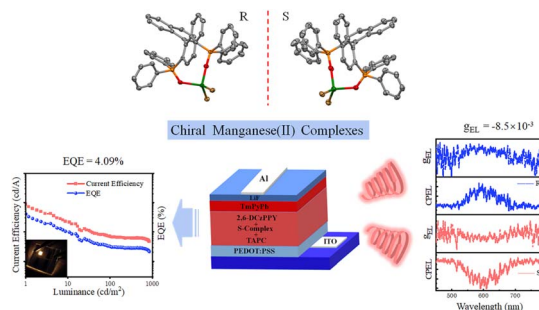
Wanlin Fu, Kuibo Yin, Zhihui Li, Jun Wang, Mingyu Tang, Jilan Tian, Litao Sun, Yueming Sun and Yunqian Dai<sup>\*</sup>



16698

### Highly efficient circularly polarized electroluminescence based on chiral manganese(II) complexes

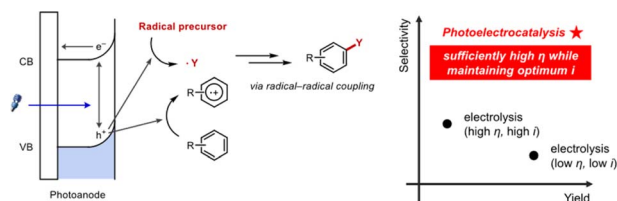
De-Hao Kong, Yue Wu, Cui-Mi Shi, Hao Zeng, Liang-Jin Xu<sup>\*</sup> and Zhong-Ning Chen<sup>\*</sup>



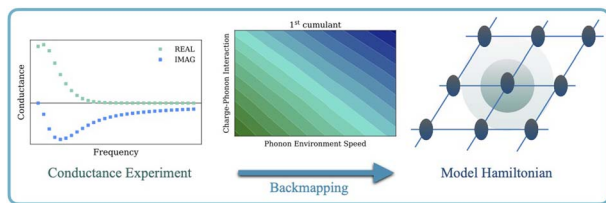
16705

### A photoelectrocatalytic system as a reaction platform for selective radical–radical coupling

Sunghwan Won, Dongmin Park, Yousung Jung,<sup>\*</sup> Hyunwoo Kim<sup>\*</sup> and Taek Dong Chung<sup>\*</sup>



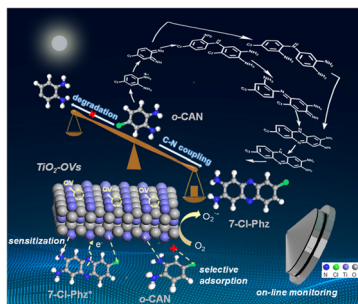
16715



## Mori generalized master equations offer an efficient route to predict and interpret polaron transport

Srijan Bhattacharyya, Thomas Sayer and Andrés Montoya-Castillo\*

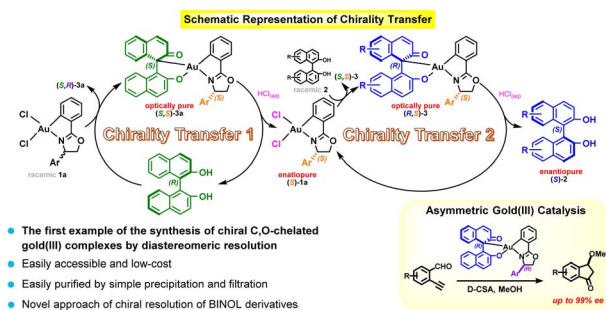
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## Competitive photooxidation of small colorless organics controlled by oxygen vacancies under visible light

Jianghui Sun, Xiyang Ge, Yixuan Gao, Min Zhang, Qi Zhao, Guohua Hou, Xiaoni Wang, Yiyang Yin, Jin Ouyang and Na Na\*

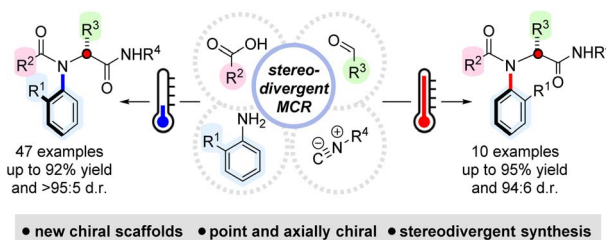
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## Consecutive chirality transfer: efficient synthesis of chiral C,O-chelated BINOL/gold(III) complexes for asymmetric catalysis and chiral resolution of disubstituted BINOLs

Kwok-Heung Aries Chan, Wa-Yi O, Jia-Jun Jiang, Jian-Fang Cui\* and Man-Kin Wong\*

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## A stereodivergent multicomponent approach for the synthesis of C–N atropisomeric peptide analogues

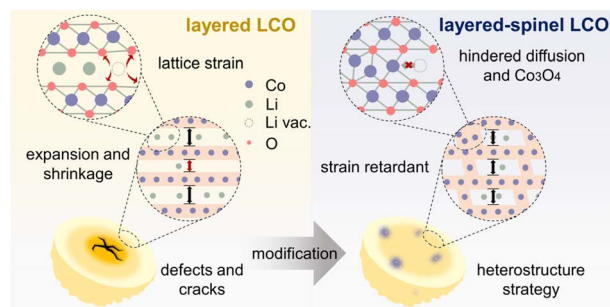
Natalie J. Roper, Aaron D. G. Campbell, Paul G. Waddell, Alistair K. Brown, Kristaps Ermanis\* and Roly J. Armstrong\*



16752

### Does “zero-strain” lithiated spinel serve as a strain retardant and an irreversible phase transition regulator for layered oxide cathodes?

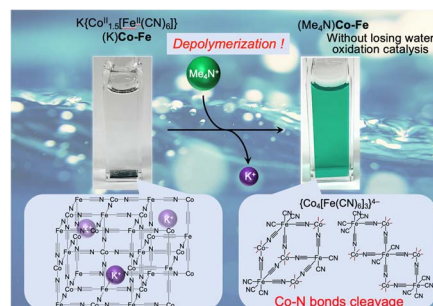
Zixin Wu, Qizheng Zheng, Guiyang Gao, Jianhua Yin, Leiyu Chen, Yonglin Tang, Yawen Yan, Huan Huang,\* Yaru Qin,\* Xiaoxiao Kuai,\* Yu Qiao\* and Shi-Gang Sun



16760

### Enhanced catalytic activity of solubilised species obtained by counter-cation exchange of K {Co<sup>II</sup><sub>1.5</sub>[Fe<sup>II</sup>(CN)<sub>6</sub>]} for water oxidation

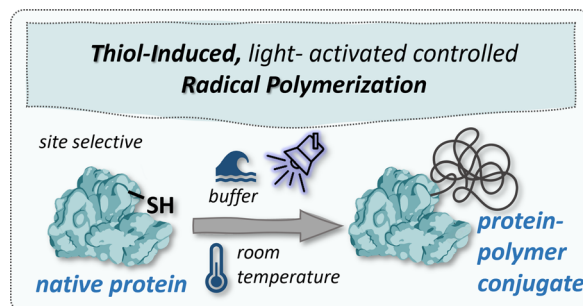
Yusuke Seki, Takashi Nakazono, Hiroyasu Tabe and Yusuke Yamada\*



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### Thiol-selective native grafting from polymerization for the generation of protein–polymer conjugates

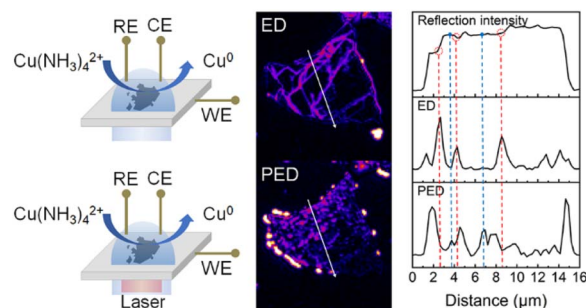
Melina I. Feldhof, Sandro Sperzel, Lorand Bonda, Susanne Boye, Adam B. Braunschweig, Ulla I. M. Gerling-Driessen\* and Laura Hartmann\*



16778

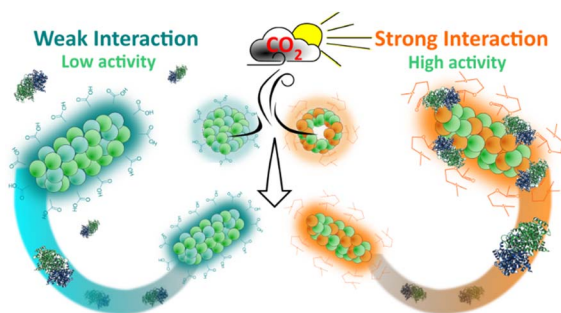
### Wide-field imaging of active site distribution on semiconducting transition metal dichalcogenide nanosheets in electrocatalytic and photoelectrocatalytic processes

Lisi Wen, Houkai Chen and Rui Hao\*





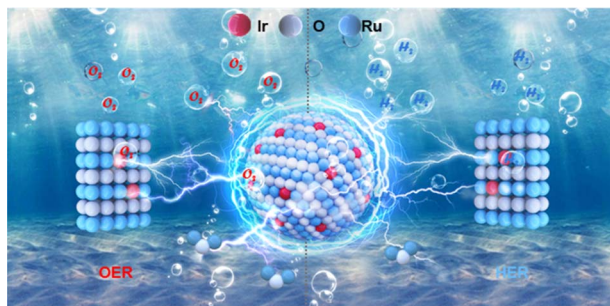
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### Photobiocatalytic CO<sub>2</sub> reduction into CO by organic nanorod-carbon monoxide dehydrogenase assemblies: surfactant matters

Mariia V. Pavliuk, Maximilian Böhm, Janna Wilhelmsen, Steffen Hardt, Henrik Land and Haining Tian\*

16796



### Dual active site-mediated Ir single-atom-doped RuO<sub>2</sub> catalysts for highly efficient and stable water splitting

Zhenhua Tao, Ning Lv, Hongyu Zhao, Xu Luo, Zilan Li, Jun Yu, Lei Chen, Xupo Liu and Shichun Mu\*

## CORRECTION

16804

### Correction: The mechanism of the molecular CISS effect in chiral nano-junctions

Thi Ngoc Ha Nguyen, Georgeta Salvan, Olav Hellwig, Yossi Paltiel, Lech Tomasz Baczewski and Christoph Tegenkamp\*

