

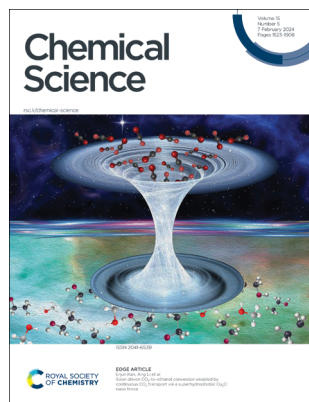
# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(5) 1523–1908 (2024)



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**Inside cover**  
See Carlos E. Puerto Galvis, Emilio Palomares *et al.*, pp. 1534–1556. Image reproduced by permission of Laia Plana Mendoza, Carlos E. Puerto Galvis and Emilio Palomares from *Chem. Sci.*, 2024, 15, 1534. Artwork by Laia Plana Mendoza and Carlos E. Puerto Galvis (ICIQ).

## PERSPECTIVES

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### Challenges in the design and synthesis of self-assembling molecules as selective contacts in perovskite solar cells

Carlos E. Puerto Galvis,\* Dora A. González Ruiz, Eugenia Martínez-Ferrero and Emilio Palomares\*

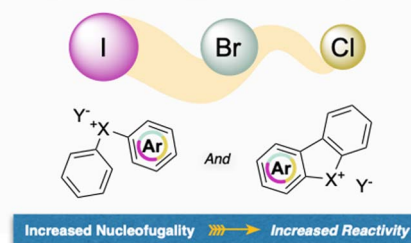


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### Diaryl hypervalent bromines and chlorines: synthesis, structures and reactivities

Matteo Lanzì\* and Joanna Wencel-Delord\*

#### Diaryl halogens hypervalent compounds



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## Energy & Environmental Science

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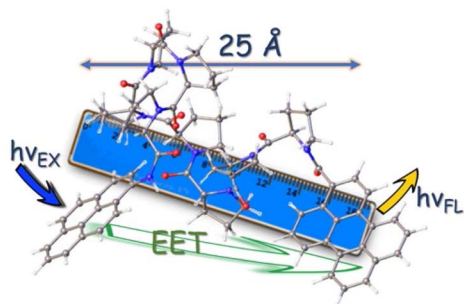
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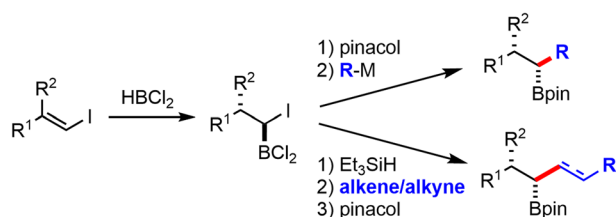
1657



### Deducing the conformational space for an octa-proline helix

Sara M. A. Waly, Andrew C. Benniston\* and Anthony Harriman\*

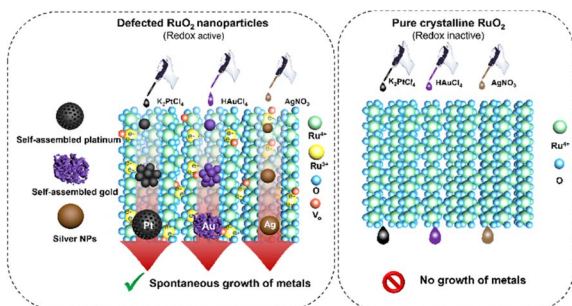
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### Borylative transition metal-free couplings of vinyl iodides with various nucleophiles, alkenes or alkynes

Gesa Seidler, Max Schwenzer, Florian Clausen, Constantin G. Daniliuc and Armido Studer\*

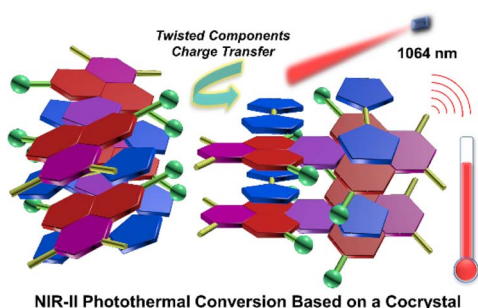
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### Hydrous ruthenium oxide triggers template-free and spontaneous growth of metal nanostructures

Faheem Muhammad, Xiwen Chen, Jiayi Tang, Yuan Cheng, Yuyang Li, Chenxin Zhu, Yihong Zhang, Leiying Miao, Yu Deng and Hui Wei\*

1692



### NIR-II photothermal conversion and imaging based on a cocrystal containing twisted components

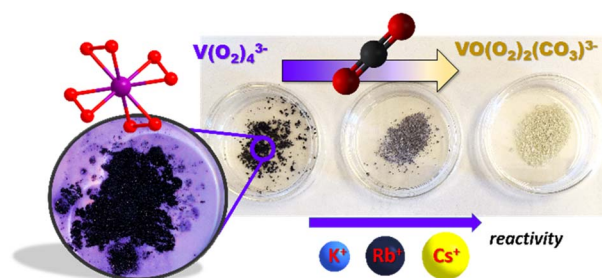
Tao Li, Jia-Chuan Liu, En-Ping Liu, Bai-Tong Liu, Jing-Yu Wang, Pei-Yu Liao, Jian-Hua Jia, Yuanning Feng\* and Ming-Liang Tong\*



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### Implementing vanadium peroxides as direct air carbon capture materials

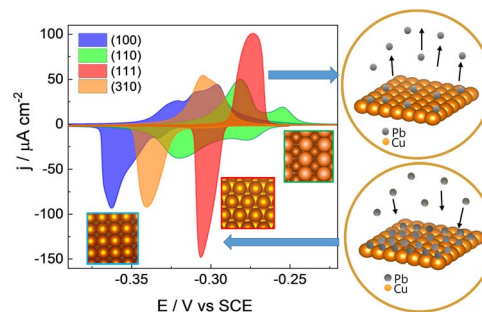
Eduard Garrido Ribó, Zhiwei Mao, Jacob S. Hirschi, Taylor Lindsay, Karlie Bach, Eric D. Walter, Casey R. Simons, Tim J. Zuehlsdorff and May Nyman\*



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### Tailoring the facet distribution on copper with chloride

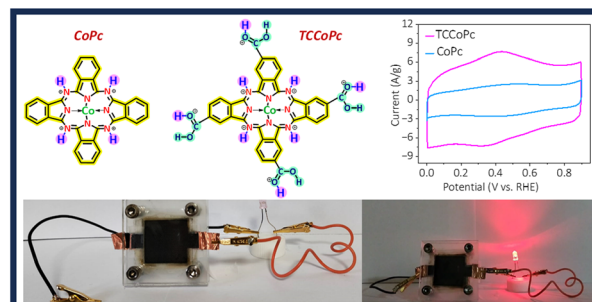
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### Electrochemical energy storage in an organic supercapacitor via a non-electrochemical proton charge assembly

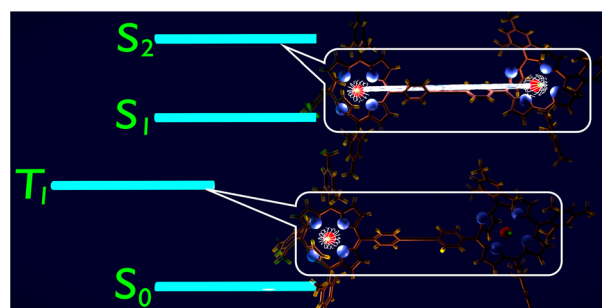
Sanchayita Mukhopadhyay, Alagar Raja Kottaichamy, Mruthyunjayachari Chattanahalli Devendrachari, Rahul Mahadeo Mendhe, Harish Makri Nimbegondi Kotresh,\* Chathakudath Prabhakaran Vinod\* and Musthafa Ottakam Thotiyal\*



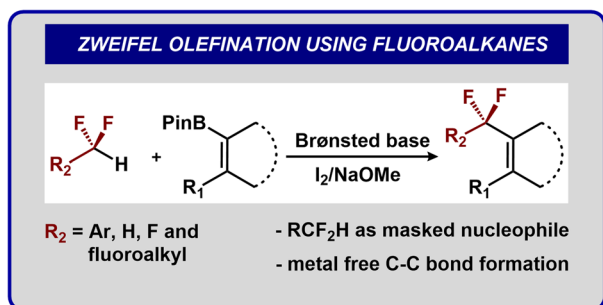
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### Decorrelated singlet and triplet exciton delocalization in acetylene-bridged Zn-porphyrin dimers

Hasini Medagedara, Mandefro Y. Teferi, Sachithra T. Wanasinghe, Wade Burson, Shahad Kizi, Bradley Zaslona, Kristy L. Mardis, Jens Niklas, Oleg G. Poluektov\* and Aaron S. Rury\*



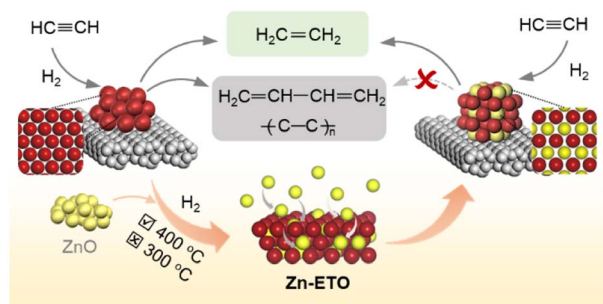
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### A metal-free strategy to construct fluoroalkyl–olefin linkages using fluoroalkanes

Kaushik Chakrabarti, Michael M. Wade Wolfe, Shuo Guo, Joseph W. Tucker, Jisun Lee and Nathaniel K. Szymczak\*

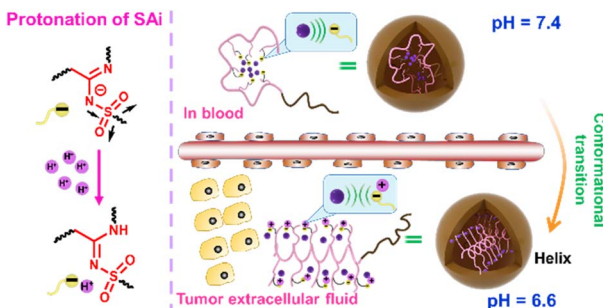
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### Thermally induced intermetallic Rh<sub>1</sub>Zn<sub>1</sub> nanoparticles with high phase-purity for highly selective hydrogenation of acetylene

Xiaocheng Lan, Yu Wang, Boyang Liu, Zhenyu Kang and Tiefeng Wang\*

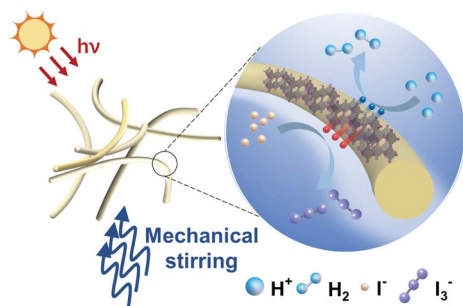
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### N-Sulfonyl amidine polypeptides: new polymeric biomaterials with conformation transition responsive to tumor acidity

Xiang Xu, Jinjuan Ma, Aiguo Wang\* and Nan Zheng\*

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### Significant hydrogen generation *via* photo-mechanical coupling in flexible methylammonium lead iodide nanowires

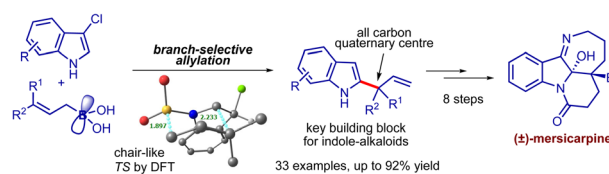
Yucheng Zhang, Jiawei Huang, Mengya Zhu, Zhouyang Zhang, Kaiqi Nie, Zhiguo Wang, Xiaxia Liao, Longlong Shu, Tingfang Tian,\* Zhao Wang,\* Yang Lu and Linfeng Fei\*



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## Construction of C2-indolyl-quaternary centers by branch-selective allylation: enabling concise total synthesis of the (±)-mersicarpine alkaloid

Minakshi Ghosh, Samrat Sahu, Shuvendu Saha and Modhu Sudan Maji\*

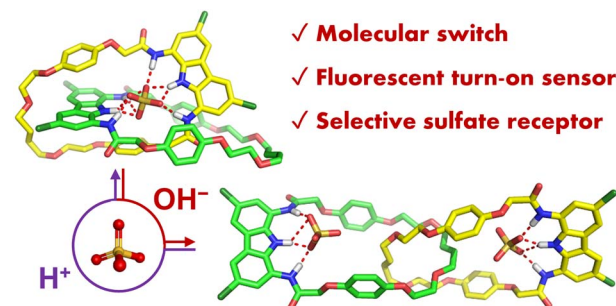


- simple allyl alcohol precursor
- excellent functional group tolerance
- scalable
- C3-unsubstituted indoles
- total synthesis of mersicarpine via two routes
- formal synthesis of (±)-scolarisine G, (±)-melodinine E, (±)-leuconoxine

1796

## Anion-templated synthesis of a switchable fluorescent [2]catenane with sulfate sensing capability

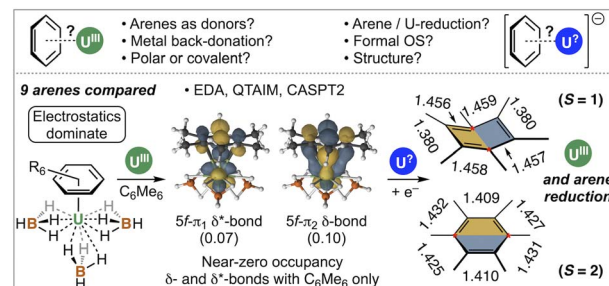
Krzysztof M. Bąk, Bartosz Trzaskowski and Michał J. Chmielewski



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## What is the nature of the uranium(III)–arene bond?

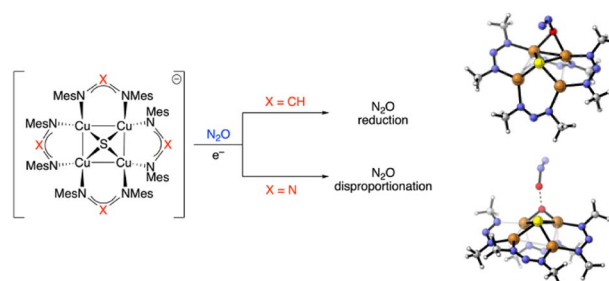
Sabyasachi Roy Chowdhury, Conrad A. P. Goodwin\* and Bess Vlaisavljevich\*



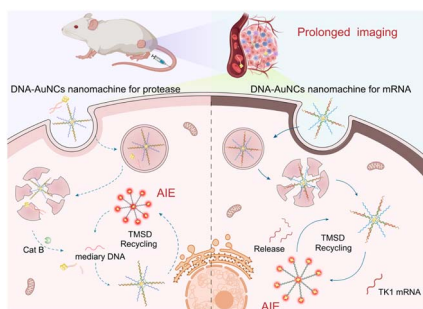
1820

## Triazenide-supported [Cu<sub>4</sub>S] structural mimics of Cu<sub>2</sub> that mediate N<sub>2</sub>O disproportionation rather than reduction

Neal P. Mankad\*



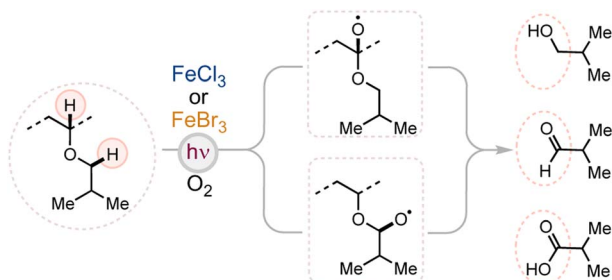
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### Prolonged near-infrared fluorescence imaging of microRNAs and proteases *in vivo* by aggregation-enhanced emission from DNA-AuNC nanomachines

Ting Wang, Kai Jiang, Yifan Wang, Limei Xu, Yingqi Liu, Shiling Zhang, Weiwei Xiong, Yemei Wang, Fenfen Zheng\* and Jun-Jie Zhu\*

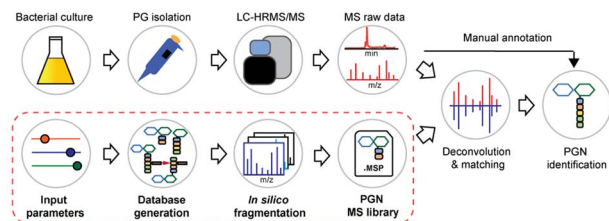
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### Selective poly(vinyl ether) upcycling via photooxidative degradation with visible light

Darren L. Langer, Sewon Oh and Erin E. Stache\*

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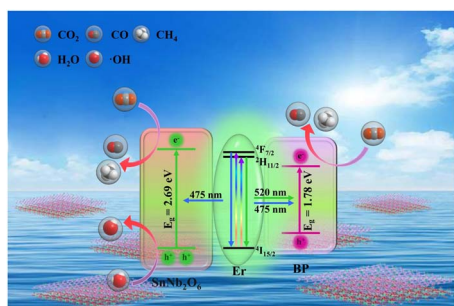


PGN\_MS2: an *in silico* PGN library for automated LC-MS/MS spectral deconvolution of bacterial peptidoglycan fragments (PGNs)

### *In silico* MS/MS prediction for peptidoglycan profiling uncovers novel anti-inflammatory peptidoglycan fragments of the gut microbiota

Jeric Mun Chung Kwan, Yaquan Liang, Evan Wei Long Ng, Ekaterina Sviriaeva, Chenyu Li, Yilin Zhao, Xiao-Lin Zhang, Xue-Wei Liu, Sunny H. Wong and Yuan Qiao\*

1860



### Study on synergistic effects of 4f levels of erbium and black phosphorus/SnNb<sub>2</sub>O<sub>6</sub> heterostructure catalysts by multiple spectroscopic analysis techniques

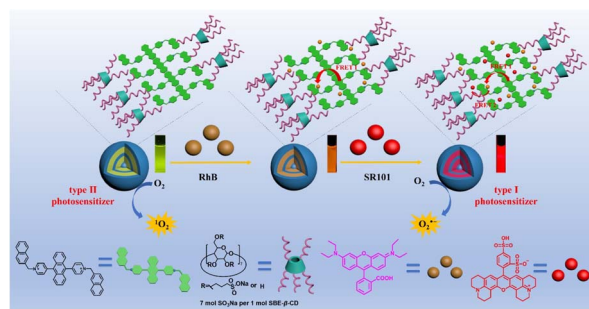
Minze Li, Jingzhen Wang, Qiuye Wang, Honglai Lu, Guofeng Wang\* and Honggang Fu\*



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### Switchover from singlet oxygen to superoxide radical through a photoinduced two-step sequential energy transfer process

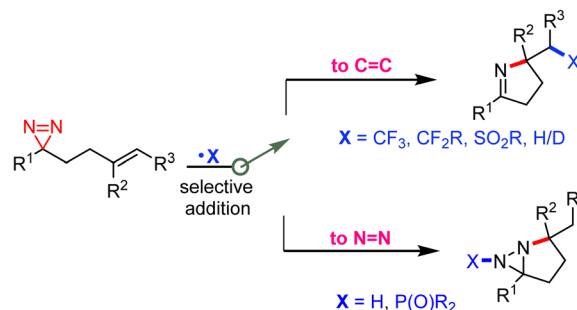
Shengsheng Yu, Rong-Xin Zhu, Kai-Kai Niu, Ning Han, Hui Liu and Ling-Bao Xing\*



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### Access to pyrrolines and fused diaziridines by selective radical addition to homoallylic diazirines

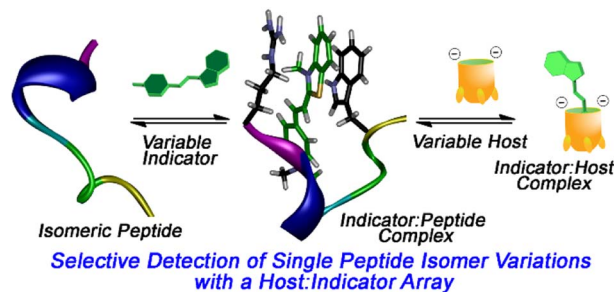
Zhigang Ma, Xinxin Wu, Haotian Li, Zhu Cao and Chen Zhu\*



1885

### Selective recognition and discrimination of single isomeric changes in peptide strands with a host: guest sensing array

Junyi Chen, Parisa Fasihianifard, Alexie Andrea P. Raz, Briana L. Hickey, Jose L. Moreno, Jr., Chia-En A. Chang, Richard J. Hooley\* and Wenwan Zhong\*



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### Electronic configuration regulation of single-atomic Mn sites mediated by Mo/Mn clusters for an efficient hydrogen evolution reaction

Chengyu Zhang, Xiangyang Wang, Renyuan Zhao, Fabrice Ndayisenga and Zhisheng Yu\*

