

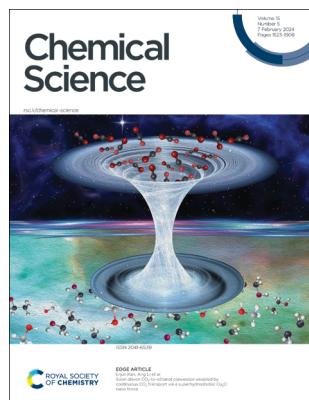
# Chemical Science

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## IN THIS ISSUE

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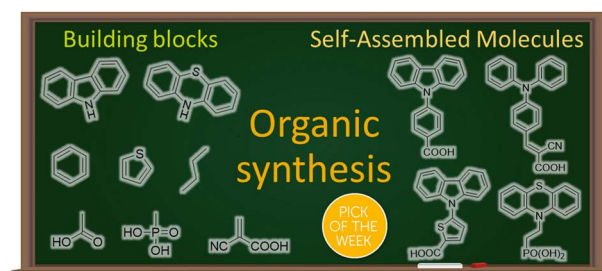
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See Carlos E. Puerto Galvis,  
Emilio Palomares *et al.*,  
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## PERSPECTIVES

1534

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

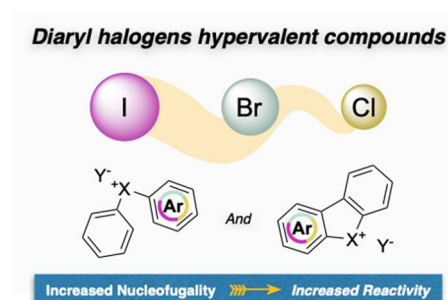
Carlos E. Puerto Galvis,\* Dora A. González Ruiz,  
Eugenia Martínez-Ferrero and Emilio Palomares\*



1557

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

Matteo Lanzi\* and Joanna Wencel-Delord\*





# Fuelling your energy research



## Energy & Environmental Science

Agenda-setting research in energy science and technology

### Chair of the Editorial Board

Jenny Nelson, Imperial College London, UK

Impact factor 2021: 39.714, median time to first decision (peer reviewed articles only): 46 days\*.

[rsc.li/ees](https://rsc.li/ees)



## EES Catalysis

Exceptional research on energy and environmental catalysis

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Driving the development of sustainable energy technologies through cutting edge research

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Garry Rumbles, National Renewable Energy Laboratory and University of Colorado Boulder, USA

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Volker Presser, Leibniz Institute for New Materials, Germany

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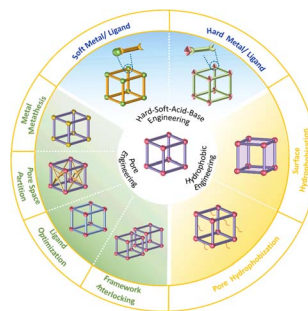


## REVIEWS

1570

**Water-stable metal–organic frameworks (MOFs): rational construction and carbon dioxide capture**

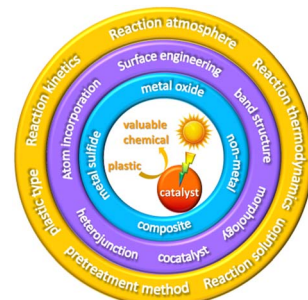
Cao Xiao, Jindou Tian, Qihui Chen\* and Maochun Hong\*



1611

**Recent advancement on photocatalytic plastic upcycling**

Jingrun Ran, Amin Talebian-Kiakalaieh, Shuai Zhang, Elhussein M. Hashem, Meijun Guo and Shi-Zhang Qiao\*

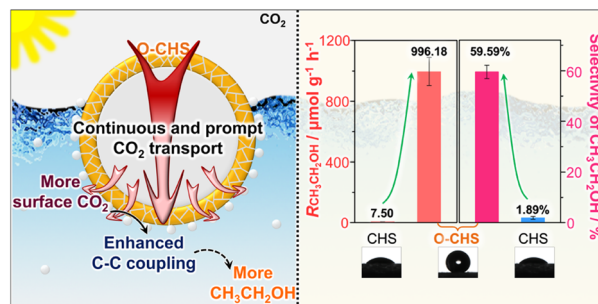


## EDGE ARTICLES

1638

**Solar-driven CO<sub>2</sub>-to-ethanol conversion enabled by continuous CO<sub>2</sub> transport via a superhydrophobic Cu<sub>2</sub>O nano fence**

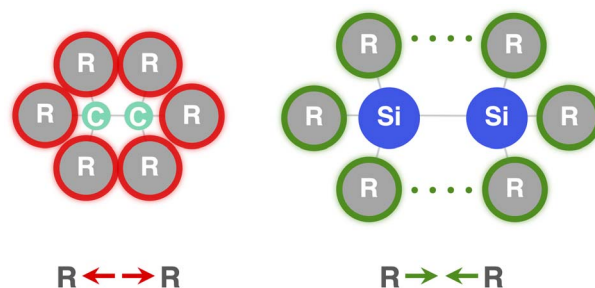
Hailing Huo, Hua He, Chengxi Huang, Xin Guan, Fang Wu, Yongping Du, Hongbin Xing, Erjun Kan\* and Ang Li\*



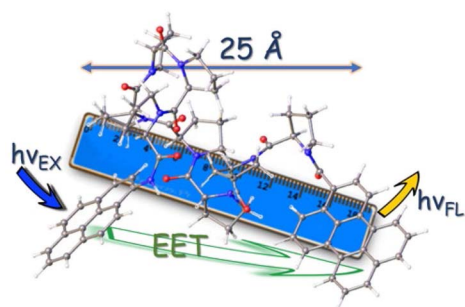
1648

**Nature and strength of group-14 A–A' bonds**

Daniela Rodrigues Silva, Eva Blokker, J. Martijn van der Schuur, Trevor A. Hamlin and F. Matthias Bickelhaupt\*



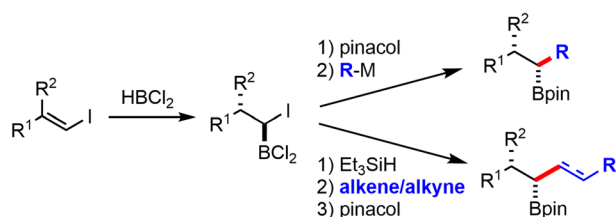
1657



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

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

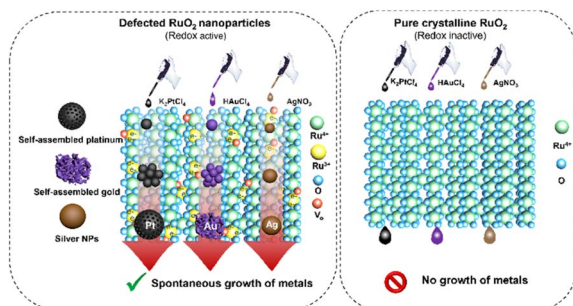
1672



### 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\*

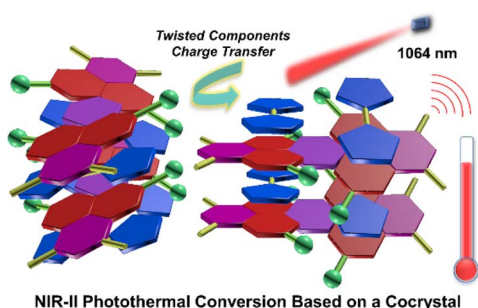
1679



### 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\*

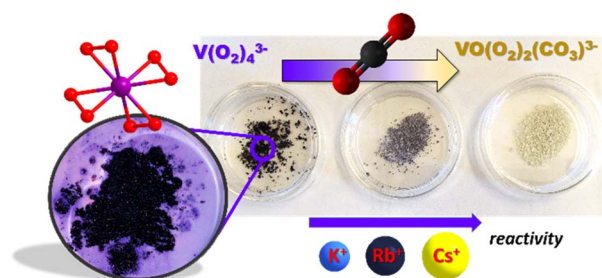




1700

## Implementing vanadium peroxides as direct air carbon capture materials

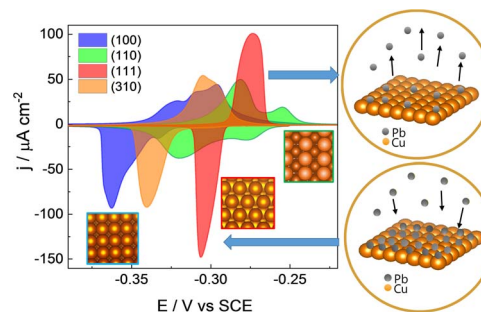
Eduard Garrido Ribó, Zhiwei Mao, Jacob S. Hirschi, Taylor Lindsay, Karlie Bach, Eric D. Walter, Casey R. Simons, Tim J. Zuehlsdorff and May Nyman\*



1714

## Tailoring the facet distribution on copper with chloride

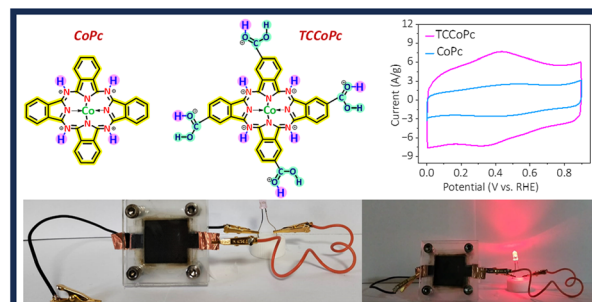
Pedro Mazaira Couce, Thor Kongstad Madsen, Elena Plaza-Mayoral, Henrik H. Kristoffersen,\* Ib Chorkendorff, Kim Nicole Dalby, Ward van der Stam, Jan Rossmeisl, María Escudero-Escribano\* and Paula Sebastián-Pascual\*



1726

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

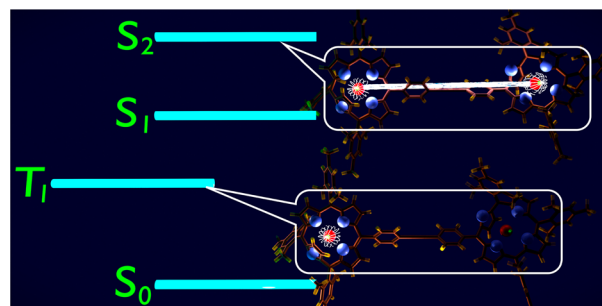
Sanchayita Mukhopadhyay, Alagar Raja Kottaichamy, Mruthyunjayachari Chattanahalli Devendrachari, Rahul Mahadeo Mendhe, Harish Makri Nimbegondi Kotresh,\* Chathakudath Prabhakaran Vinod\* and Musthafa Ottakam Thotiyi\*



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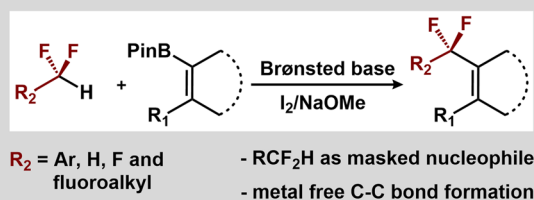
## Decorrelated singlet and triplet exciton delocalization in acetylene-bridged Zn-porphyrin dimers

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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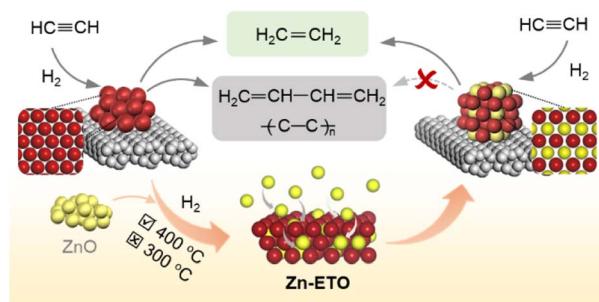
## ZWEIFEL OLEFINATION USING FLUOROALKANES



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

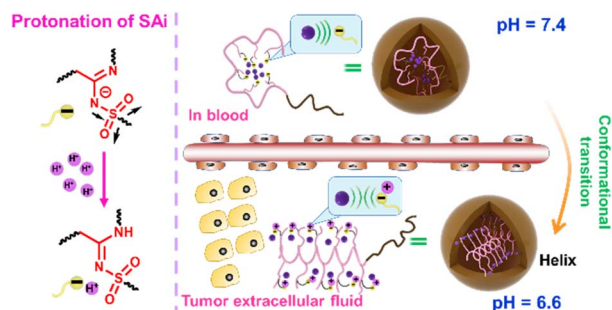
Kaushik Chakrabarti, Michael M. Wade Wolfe, Shuo Guo, Joseph W. Tucker, Jisun Lee and Nathaniel K. Szymczak\*

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Thermally induced intermetallic  $\text{Rh}_1\text{Zn}_1$  nanoparticles with high phase-purity for highly selective hydrogenation of acetylene

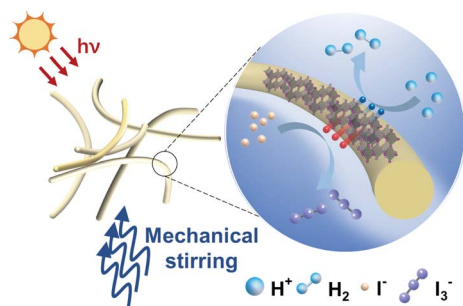
Xiaocheng Lan, Yu Wang, Boyang Liu, Zhenyu Kang and Tiefeng Wang\*

1769

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

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

1782

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\*





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

1796

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

✓ Molecular switch  
 ✓ Fluorescent turn-on sensor  
 ✓ Selective sulfate receptor

H<sup>+</sup> OH<sup>-</sup>

## 1810

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

- Arenes as donors?
- Metal back-donation?
- Polar or covalent?

• Arene / U-reduction?  
 • Formal OS?  
 • Structure?

**9 arenes compared**

- EDA, QTAIM, CASPT2

Electrostatics dominate

$R_6$

$C_6Me_6$

$5f\pi_1 \delta^* \text{-bond}$   
 (0.07)

$5f\pi_2 \delta^* \text{-bond}$   
 (0.10)

Near-zero occupancy  
 $\delta^-$  and  $\delta^+$ -bonds with  $C_6Me_6$  only

$U^{IV}$   
 $+ e^-$

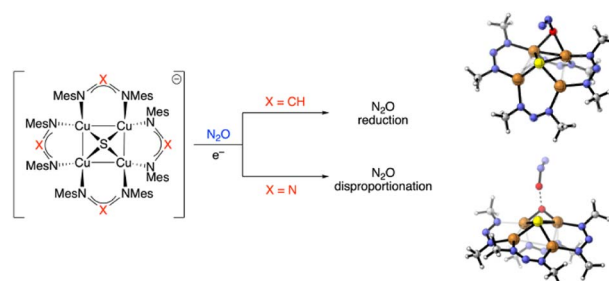
and arene reduction

$(S = 1)$

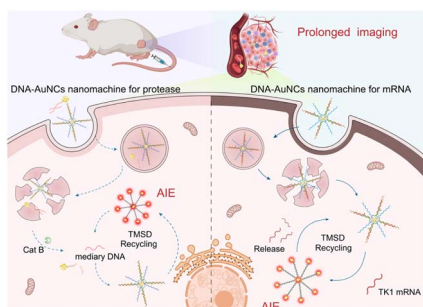
$(S = 2)$

## 1820

## Neal P. Mankad\*



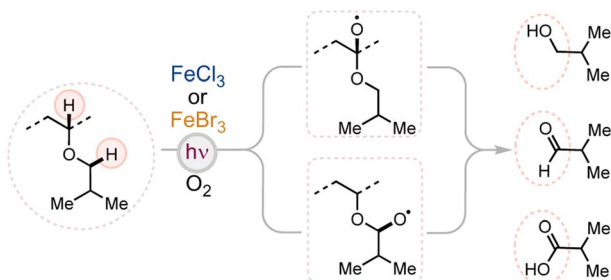
1829



### 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\*

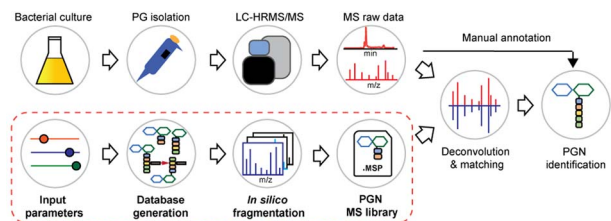
1840



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

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

1846

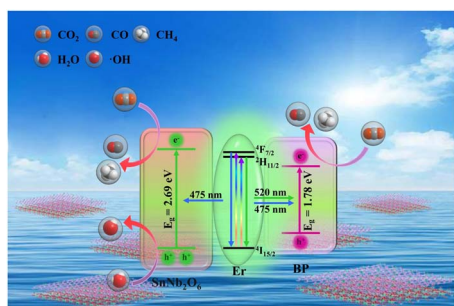


PGN\_MS2: an *in silico* PGN library for automated LC-MS/MS spectral deconvolution of bacterial peptidoglycan fragments (PGNs)

### *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\*

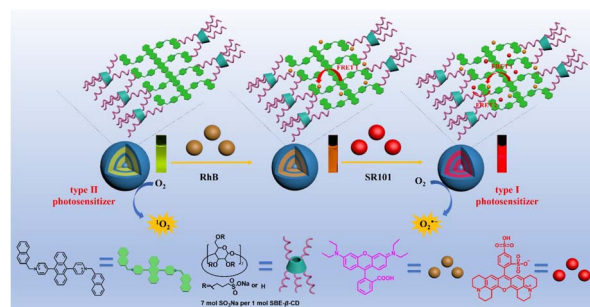




1870

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

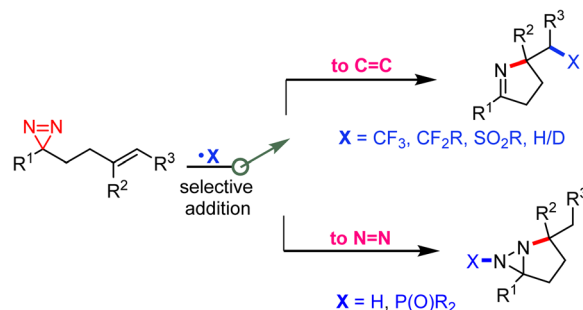
Shengsheng Yu, Rong-Xin Zhu, Kai-Kai Niu, Ning Han, Hui Liu and Ling-Bao Xing\*



1879

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

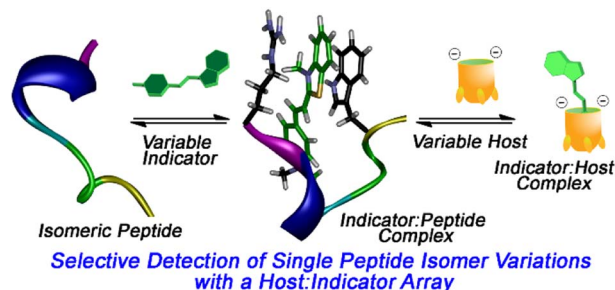
Zhigang Ma, Xinxin Wu, Haotian Li, Zhu Cao and Chen Zhu\*



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\*



1894

## 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\*

