

# Chemical Science

rsc.li/chemical-science

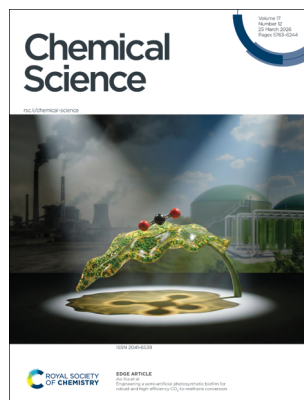
The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 17(12) 5763–6244 (2026)



**Cover**  
See Hao Li *et al.*,  
pp. 5782–5804.  
Image reproduced by  
permission of Hao Li from  
*Chem. Sci.*, 2026, 17, 5782.



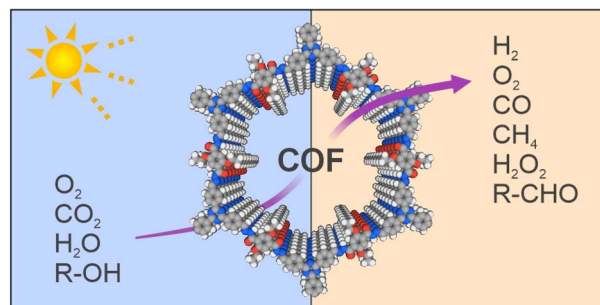
**Inside cover**  
See Ao Xia *et al.*,  
pp. 5857–5868.  
Image reproduced by  
permission of Huize Chen  
from *Chem. Sci.*,  
2026, 17, 5857.

## COMMENTARY

5777

### A reflection on 'A hydrazone-based covalent organic framework for photocatalytic hydrogen production': teaching sponges new tricks

Andrés Rodríguez-Camargo and Bettina V. Lotsch\*

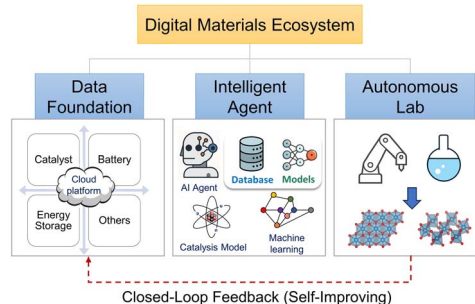


## PERSPECTIVES

5782

### Digital materials ecosystem: from databases to AI agents for autonomous discovery

Di Zhang, Xue Jia, Yuhang Wang, Heng Liu, Qian Wang, Seong-Hoon Jang, Daksh Shah, Songbo Ye, Hung Ba Tran and Hao Li\*



# Royal Society of Chemistry approved training courses

Explore your options.  
Develop your skills.  
Discover learning  
that suits you.

**Courses in the classroom,  
the lab, or online**

Find something for every  
stage of your professional  
development. Search our  
database by:

- subject area
- location
- event type
- skill level

Members **get at least 10% off**

Visit [rsc.li/cpd-training](https://rsc.li/cpd-training)



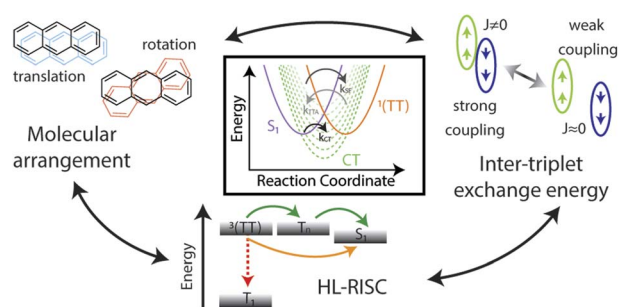
**SAVE  
10%**

## PERSPECTIVES

5805

## Controlling the fate of two triplet states: solid-state annihilator design for photon upconversion

Jussi Isokuortti\* and Lea Nienhaus\*

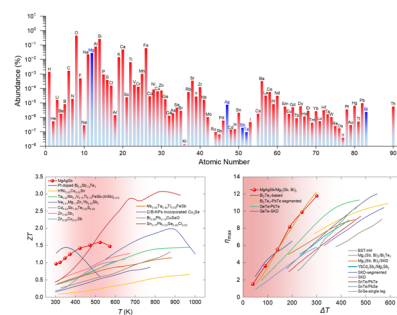


## REVIEWS

5820

## Advances in MgAgSb thermoelectrics: from materials to devices

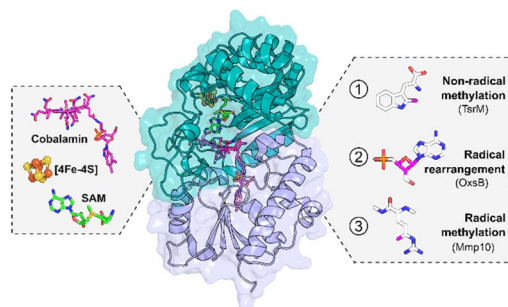
Liangjun Xie, Ran He,\* Jiehe Sui, Kornelius Nielsch and Zihang Liu\*



5840

Novel chemistry and structural perspectives in vitamin B<sub>12</sub>-dependent radical SAM enzymes

Olivier Berteau,\* Magda Teixeira Nunes, Nicole Taraglio, Pierre Legrand and Alhosna Benjdia\*

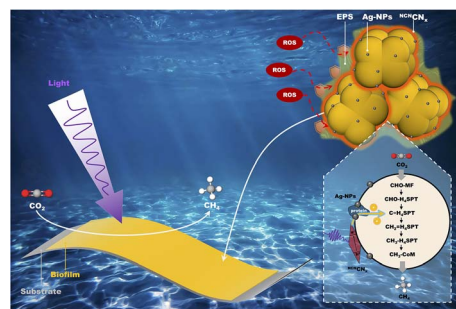


## EDGE ARTICLES

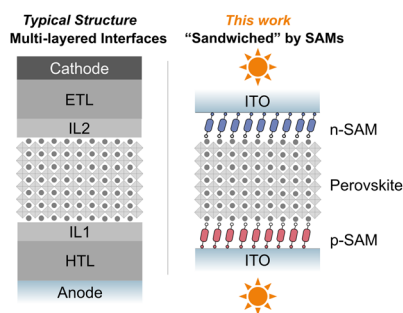
5857

Engineering a semi-artificial photosynthetic biofilm for robust and high-efficiency CO<sub>2</sub>-to-methane conversion

Huize Chen, Ao Xia,\* Yun Huang, Junyi Ji, Jingmiao Zhang, Xianqing Zhu, Xun Zhu and Qiang Liao



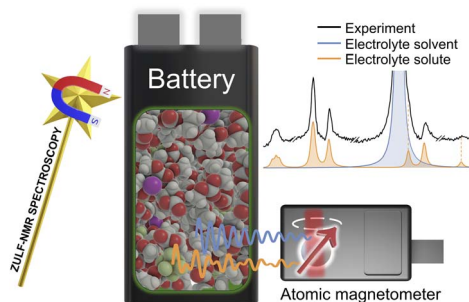
5869



## All-SAM interfacial architecture for perovskite solar cells without charge transport materials

Zhanhao Hu, Nao Saito, Masashi Ikegami,  
Naoyuki Shibayama\* and Tsutomu Miyasaka\*

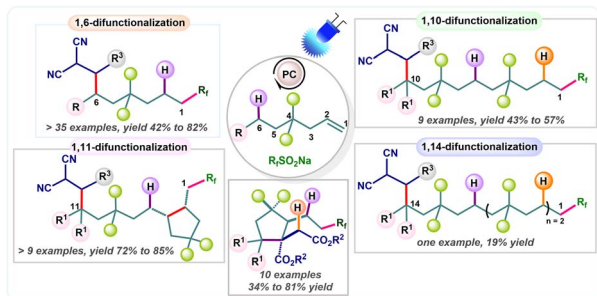
5877



## Enabling nondestructive observation of electrolyte composition in batteries with ultralow-field nuclear magnetic resonance

Anne M. Fabricant, Román Picazo-Frutos, Florin Teleanu,  
Gregory J. Rees, Raphael Kircher, Mengjiang Lin,  
William Evans, Paul-Martin Luc, Robert A. House,  
Peter G. Bruce, Peter Krüger, John W. Blanchard,  
James Eills, Kirill F. Sheberstov, Rainer Körber,  
Dmitry Budker,\* Danila A. Barskiy and Alexej Jerschow\*

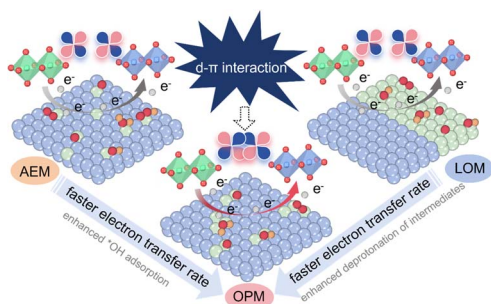
5888



## Photocatalytic remote C(sp<sup>3</sup>)-H alkylation of long-chain alkenes: A tandem multicomponent approach via radical translocation

Krishna Gopal Ghosh, Debabrata Das, Vinjamuri Srinivasu,  
Koustav Pal and Devarajulu Sureshkumar\*

5899



## Unveiling structural forms of Ru in WO<sub>x</sub>-template catalysts for efficient acidic PEM water electrolysis

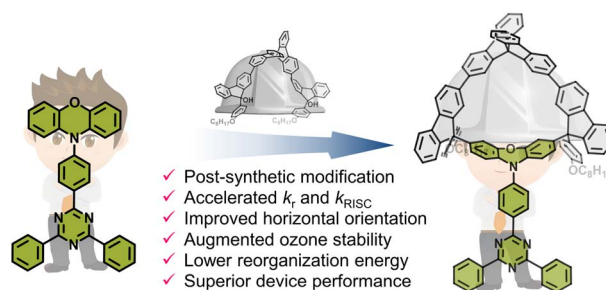
Xiongfeng Zeng, Ao Cai, Junhui Pei, GuiXin Liu, WenLu Li,  
Xiaoman Xiong,\* Ding Zhou\* and Na Yao\*



5911

### Post-synthetic gridization enhances spin-flip dynamics, horizontal alignment, and ozone resistance in solution-processable TADF macrocycles

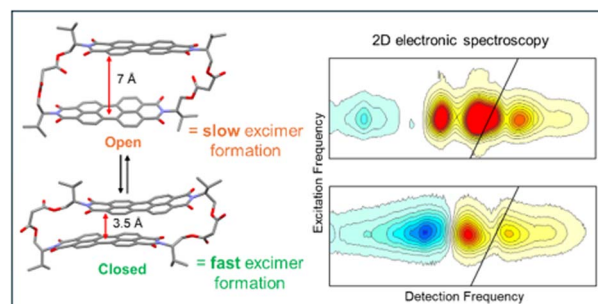
Quanyou Feng, Aiyun Zhu, Qiuhan Han, Kewei Guo, Yunfei Zhu, Yue Cao, Jingyao Ma, Hao Li, Hongjian Wang, Yuyu Pan,\* Xinxin Ban, Mengna Yu, Man Xu, Zilu Wang,\* Guohua Xie, Linghai Xie\* and Wei Huang\*



5921

### Conformational switching modulates excited-state pathways in a cofacial perylene dimer

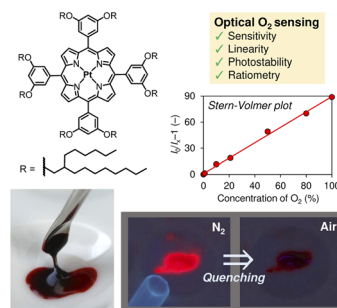
Giovanni Bressan,\* Denis Hartmann, Jonathan Brouwer, Erico M. Braun, James N. Bull and Timothy A. Barendt\*



5934

### Luminescent core-isolated solvent-free liquids as a soft material platform for optical gas sensing

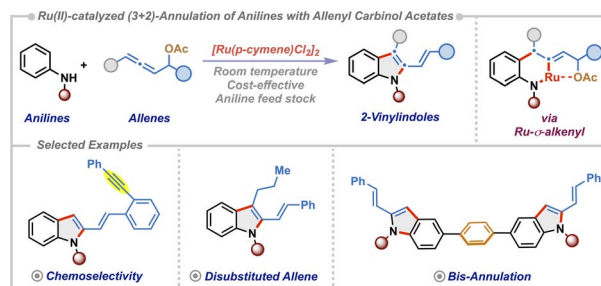
Shinsuke Ishihara,\* Avijit Ghosh, Tatsuya Mori, Mandeep K. Chahal, Daniel T. Payne, Akinori Saeki, Tsuyoshi Hyakutake and Takashi Nakanishi\*



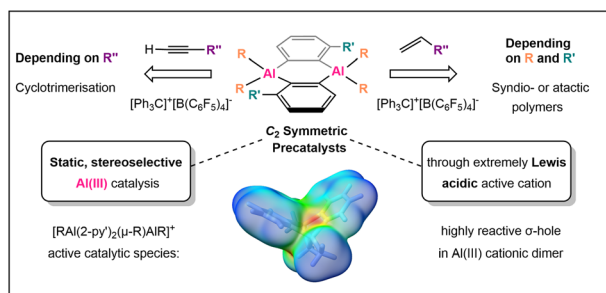
5944

### Ru(II)-catalyzed regioselective (3 + 2)-annulation of anilines with allenes to access 2-vinylindoles

Om Prakash Dash, Anurag Singh, Rahul K. Shukla and Chandra M. R. Volla\*



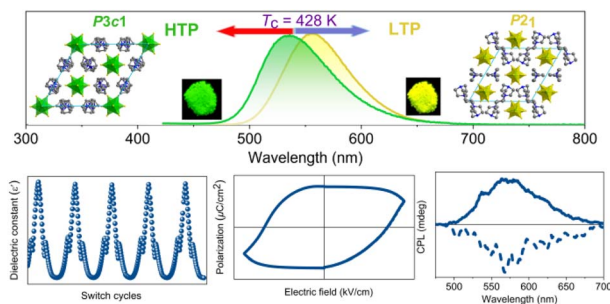
5953



### Oligomerisation and stereoselective polymerisation of alkenes and alkynes using pyridyl-based Al(III) catalysts

Dipanjana Choudhury, Richard Danylyuk, Alexandros Terzopoulos, Natalie S. Potter, Oren A. Scherman,\* Jonathan M. Goodman\* and Dominic S. Wright\*

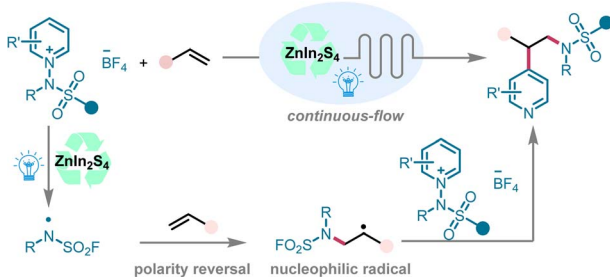
5965



### Rotational symmetry dication assembling ferroelectric, thermochromic and circularly polarized luminescent multifunctional manganese(II) bromide hybrid

Jiayi Yuan, Yu Xu, Lu Zhai,\* Shan-Shan Hei, Jianyi Huang, Weihua Ning,\* Hong-Ling Cai\* and Xiao-Ming Ren\*

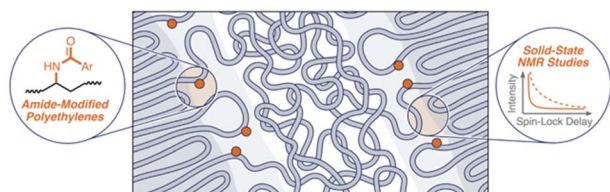
5972



### Heterogeneous photocatalytic C4 remote fluorosulfonamidation of pyridines

Panjie Xiang, Kai Sun,\* Xiaolan Chen,\* Kang Li, Xi Chen, Yunkai Zhang, Lingbo Qu and Bing Yu\*

5984



### Microstructure of amide-functionalized polyethylenes determined by NMR relaxometry

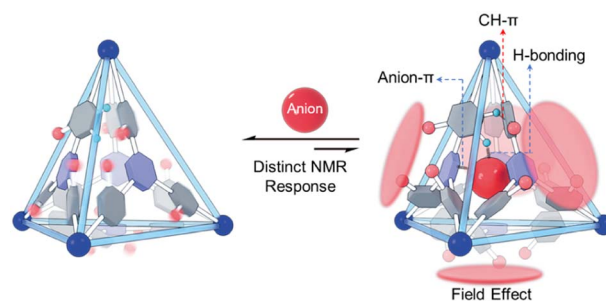
Shira Haber,\* Nicodemo R. Ciccio, Zhengxing Peng, Feipeng Yang, Julia Im, Mutian Hua, Sophia N. Fricke, Raynald Giovine, Brett A. Helms, Cheng Wang, John F. Hartwig\* and Jeffrey A. Reimer\*



5993

### Neutral anion-detecting organic cages based on anion- $\pi$ interactions

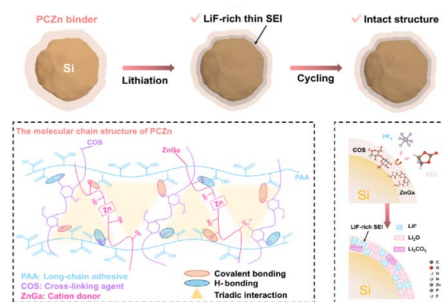
Yuyang Lu, Ping Zhou, Hua Tang, Yating Wu, Yueyan Kuang, Ze Cao, Jiyong Liu, Guangcheng Wu,\* Hongliang Chen\* and Hao Li\*



6005

### A fluorine-absorbing and mechanically elastic binder with triangular architecture enables both bulk- and interface-stable Si anodes

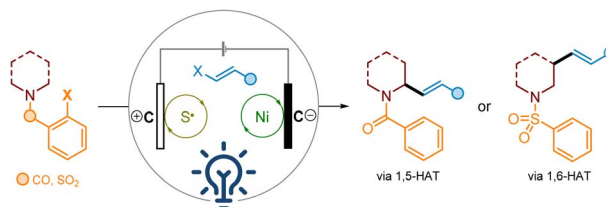
Zhipeng Wang, Qitao Shi,\* Weiqi Song, Luwen Li, Jiaqi Wang, Cheng Zhang, Alicja Bachmatiuk, Chen Lu, Peichao Zou,\* Jinho Choi,\* Yanbin Shen,\* Ruizhi Yang\* and Mark H. Rummeli\*



6017

### Remote $\alpha$ - and $\beta$ -C(sp<sup>3</sup>)-H alkenylation of amines via visible-light supported paired electrolysis

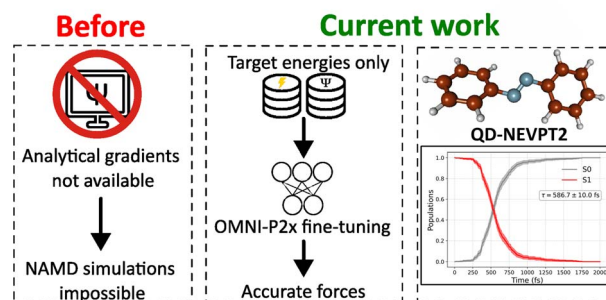
Siddharth K. Dave and Sebastian Stecko\*



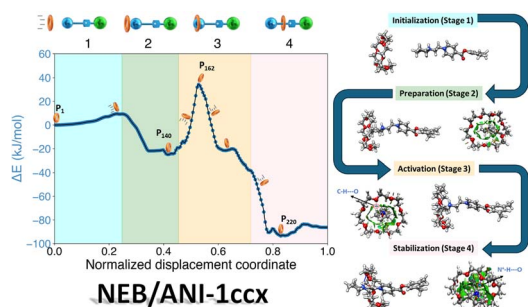
6043

### Gradients not needed: ML-driven propagation of nonadiabatic molecular dynamics without reference gradients

Mikołaj Martyka, Joanna Jankowska,\* Hans Lischka\* and Pavlo O. Dral\*



6055



### The interlocking process in molecular machines explained by a combined approach: the nudged elastic band method and machine learning potential

Lucio Peña-Zarate, Alberto Vela\* and Jorge Tiburcio\*

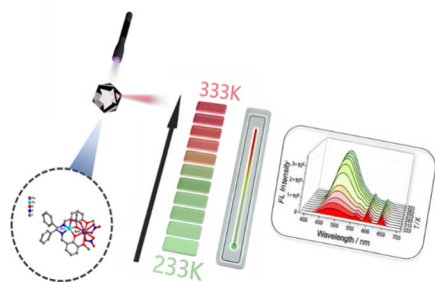
6068



### Electrostatic decatalysis through coulombic screening

Bhojkumar Nayak, Abdul Raafik Arattu Thodika, Hemanga Pradhan, Rahul Mahadeo Mendhe and Musthafa Ottakam Thotiyil\*

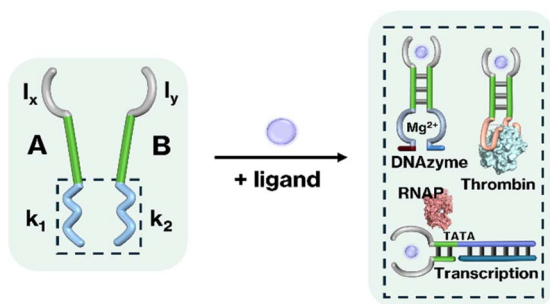
6079



### A molecular dual-center emitter for ratiometric optical thermometry

Rong Sun, Hong Huang, Ye Xia, Youchao Liu, Xingquan Tao, Jun-Long Zhang, Bing-Wu Wang\* and Song Gao\*

6086



### Allosteric ligand-aptamer complexes orchestrate supramolecular or transient catalytic, transcription and fibrinogenesis processes

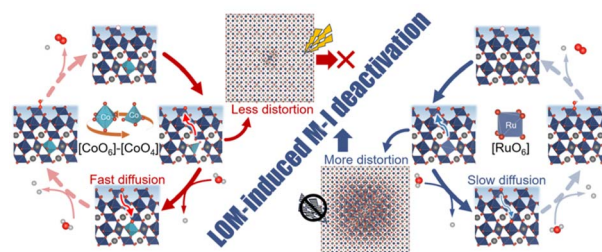
Diva Froim, Hadar Amartely, Jiantong Dong,\* Eli Pikarsky and Itamar Willner\*



6099

### Cobalt-mediated structural transition: facilitating rapid synthesis and enhanced performance of pyrochlore materials for efficient water electrolysis

Yanzong Huang, Tongtong Liu, Qingren Zhang, Yanfei Wang,\* Zhengping Zhang\* and Feng Wang\*

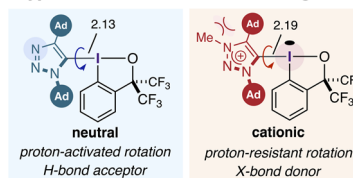


6109

### Carbon–iodine atropisomerism on triazole and triazolium frameworks: a breathing axle with divergent adaptivity

Ryoga Nambu, Jun Kikuchi,\* Arimasa Matsumoto\* and Naohiko Yoshikai\*

#### Hypervalent rotors with a "breathing" axle



$\Delta G^{\ddagger}_{rot} \sim 29 \text{ kcal mol}^{-1}$ ,  $t_{1/2 \text{ rac}} \sim 6 \text{ y}$

Facile synthesis via CuAAC

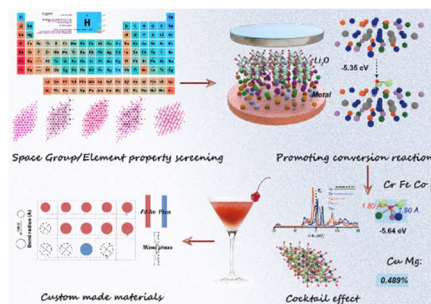
Backbone-encoded asymmetry

Divergent response & recognition

6116

### Deciphering functional differentiation of elements in high-entropy spinel oxides as ultralong-life anodes in lithium-ion batteries

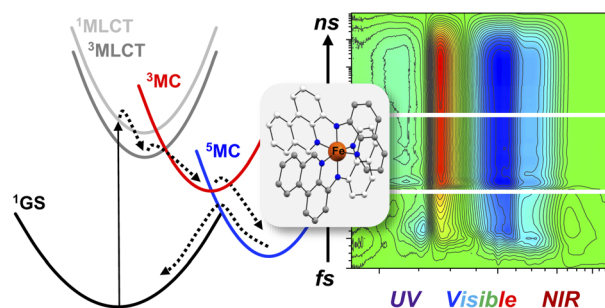
Han-Hao Liu, Jia-Lin Yang, Zhen-Yi Gu,\* Yue Liu, Xiao-Tong Wang, Chuan-Yu Zheng, Changshan Xu, Dai-Huo Liu, Wei Guo\* and Xing-Long Wu\*



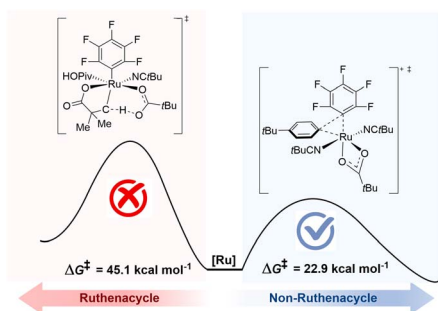
6125

### Resolving consecutive excited-state evolution in Fe-amido chromophores by wide-band optical transient absorption spectroscopy

Christina Wegeberg, Baldeep K. Sidhu, Pavel Chábera, Jens Uhlig, Rory A. Cowin, Julia A. Weinstein, Petter Persson,\* Arkady Yartsev\* and David E. Herbert\*



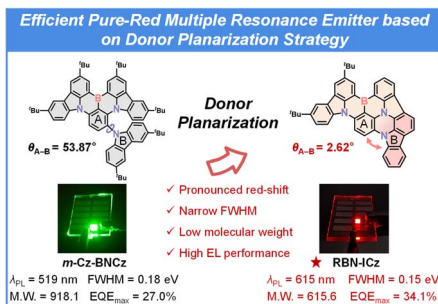
6138



### Undirected ruthenium-catalyzed C–H activation using arylsulfonium salts: direct arylation without ruthenacycle intermediates revealed by computation and data science

Jinbin Zhu, Binbin Yuan, Xuexue Chang, Hasret Can Gülen and Lutz Ackermann\*

6147



### Efficient pure-red multiple resonance emitter based on a donor planarization strategy

Linjie Li, Yincai Xu,\* Dongyue Zhang, Yupei Qu, Yue Wang and Chenglong Li\*

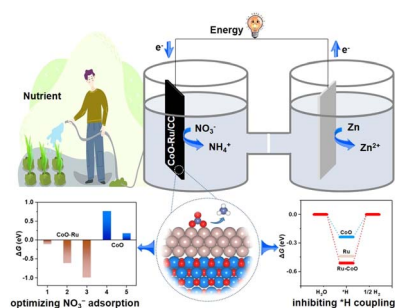
6156



### Electron spectroscopy for chemical analysis of liquids

Lukáš Tomaník,\* Florian Trinter, Petr Slaviček and Bernd Winter\*

6165



### Nanoscale Ru unlocking nanoneedles assembled into hierarchical CoO microspheres for efficient nitrate-to-ammonia electroconversion

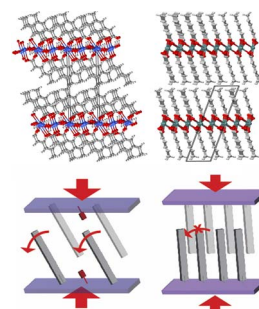
Jinxiu Zhao, Xuejing Liu, Xiang Ren,\* Dan Zhao, Zhen Li, Qing Kang, Chang-wen Zhang, Linrui Hou, Qin Wei\* and Changzhou Yuan\*



6178

### Making room for reactivity in topochemical transformations under pressure

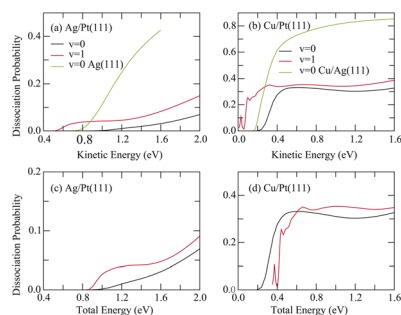
Tengteng Lyu, Jonathan B. Lefton, Martin Etter, Shrikant Bhat, Wenhao Liu, Bing Lv, Luke J. Kwan, Hao Yan\* and Tomče Runčevski\*



6187

### Harnessing work-function-driven rotational steering for quantum state control in HCl dissociation on bimetallic alloys

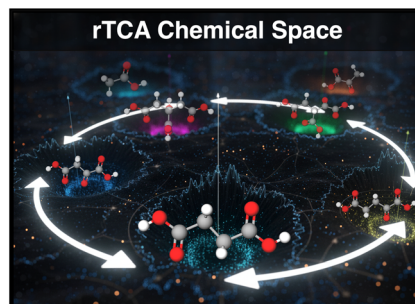
Tianhui Liu\* and Kaixin Meng



6197

### Kinetics overcome thermodynamics in primitive analogs of the reverse tricarboxylic acid cycle

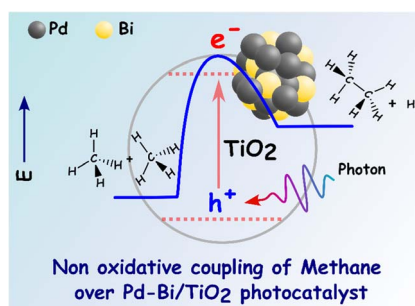
Vignesh Sathyaseelan, John Morgan\* and Brett M. Savoie\*



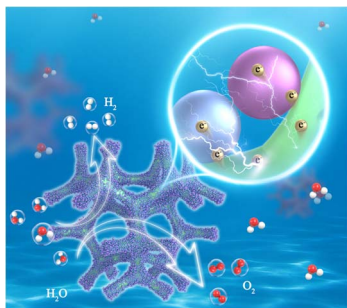
6208

### Nonoxidative coupling of methane to ethane over a Pd–Bi deposited titania photocatalyst in a flow reactor

Preetam Dash, Yuan Zhong, Daichi Takami, Akira Yamamoto and Hisao Yoshida\*



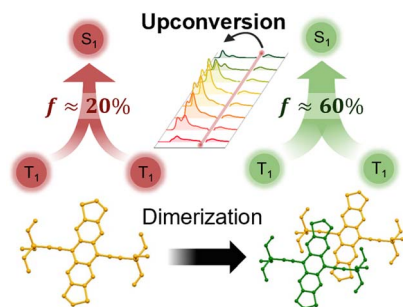
6220



### Electron enrichment enables RuPd to achieve 1.406 V overall water splitting

Yuqin Yin, Hongyu Zhao, Zhanghu Yu, Guanren Ge, Shiyuan Feng, Haoyu Zhou, Kaiyang Sun, Jie Du, Tong Chen, Zhihao Yang, Jun Yu\* and Shichun Mu\*

6230



### Aggregation favors singlet formation in TES-ADT triplet annihilator for photon upconversion

Justas Lekavičius, Edvinas Radiunas, Gediminas Kreiza, Augustina Jozeliūnaitė, Edvinas Orentas and Karolis Kazlauskas\*

6238

### Correction: Rotational symmetry dication assembling ferroelectric, thermochromic and circularly polarized luminescent multifunctional manganese(II) bromide hybrid

Jiayi Yuan, Yu Xu, Lu Zhai,\* Shan-Shan Hei, Jianyi Huang, Weihua Ning,\* Hong-Ling Cai\* and Xiao-Ming Ren\*

6239

### Correction: Enantioselective C(sp<sup>3</sup>)-H bond functionalization enabled by Cp<sup>x</sup>M(III) catalysis (M = Co, Rh, Ir)

Shu-Bin Mou, Mu-Peng Luo, Feifei Fang, Shi Cao,\* Dong Wu\* and Shou-Guo Wang\*

