

# Chemical Science

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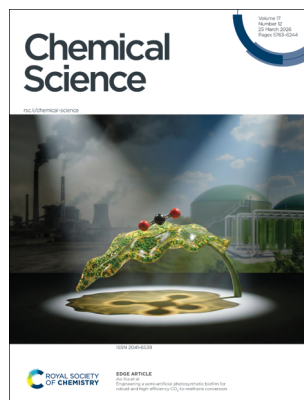
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## IN THIS ISSUE

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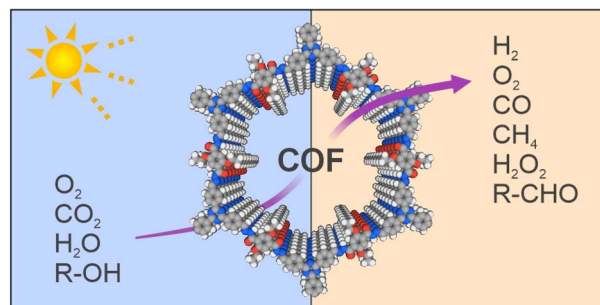
**Inside cover**  
See Ao Xia *et al.*,  
pp. 5857–5868.  
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2026, 17, 5857.

## 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\*

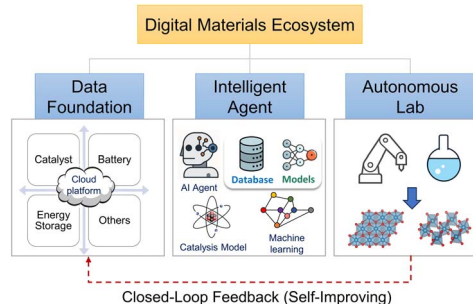


## PERSPECTIVES

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\*



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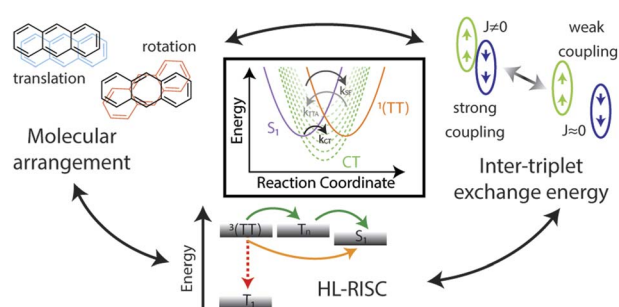
**SAVE  
10%**

## PERSPECTIVES

5805

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

Jussi Isokuortti\* and Lea Nienhaus\*

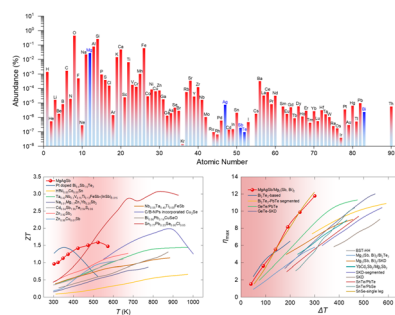


## REVIEWS

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## Advances in MgAgSb thermoelectrics: from materials to devices

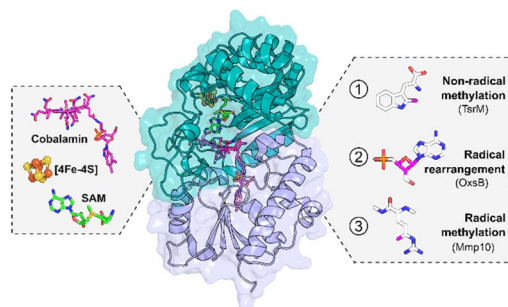
Liangjun Xie, Ran He,\* Jiehe Sui, Kornelius Nielsch and Zihang Liu\*



5840

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

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

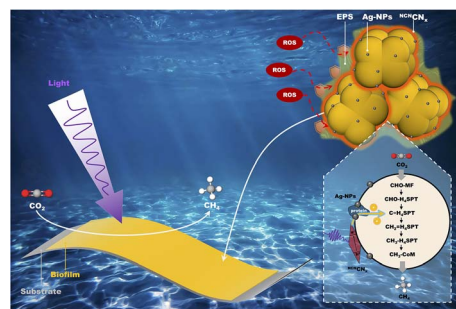


## EDGE ARTICLES

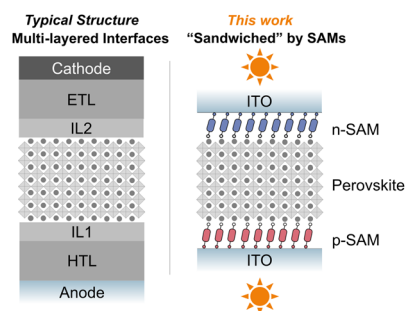
5857

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



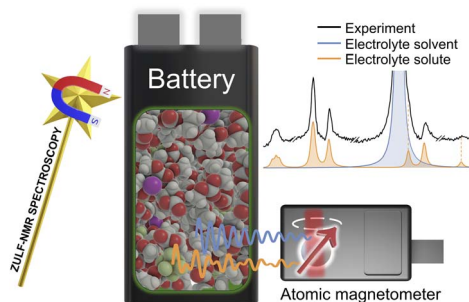
5869



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

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

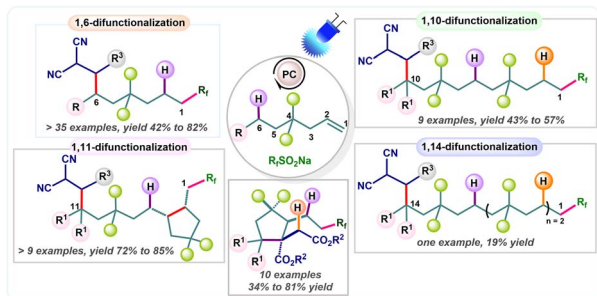
5877



## 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\*

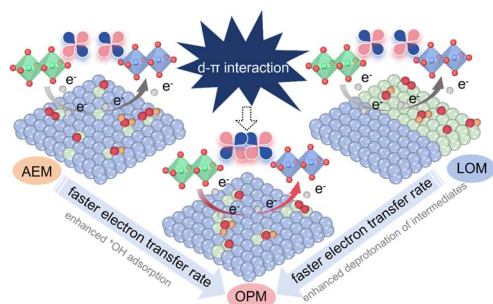
5888



## 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

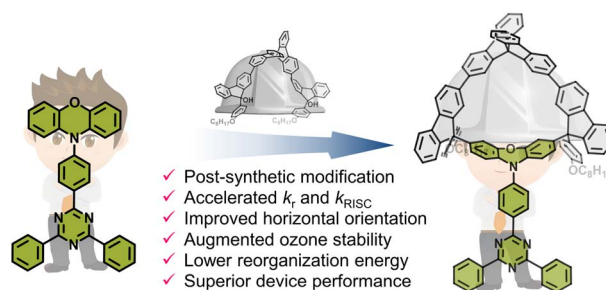
Xiongfeng Zeng, Ao Cai, Junhui Pei, GuiXin Liu, WenLu Li,  
Xiaoman Xiong,\* Ding Zhou\* and Na Yao\*



5911

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

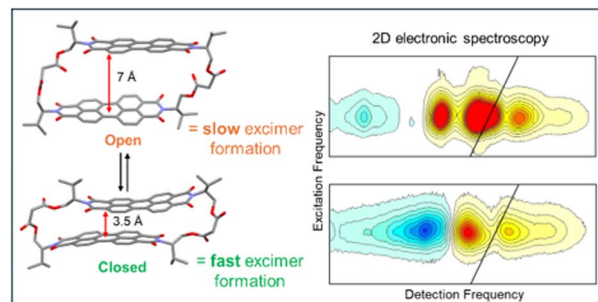
Quanyou Feng, Aiyun Zhu, Qiuhan Han, Kewei Guo, Yunfei Zhu, Yue Cao, Jingyao Ma, Hao Li, Hongjian Wang, Yuyu Pan,\* Xinxin Ban, Mengna Yu, Man Xu, Zilu Wang,\* Guohua Xie, Linghai Xie\* and Wei Huang\*



5921

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

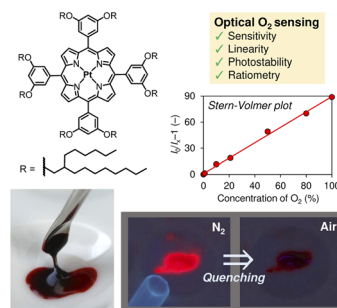
Giovanni Bressan,\* Denis Hartmann, Jonathan Brouwer, Erico M. Braun, James N. Bull and Timothy A. Barendt\*



5934

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

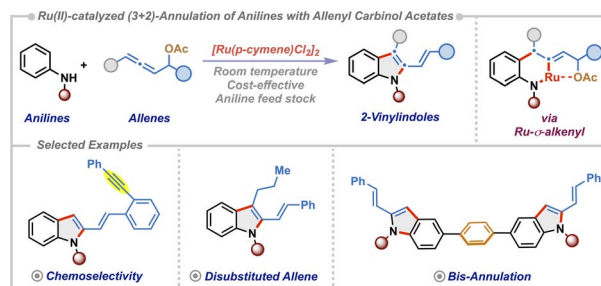
Shinsuke Ishihara,\* Avijit Ghosh, Tatsuya Mori, Mandeep K. Chahal, Daniel T. Payne, Akinori Saeki, Tsuyoshi Hyakutake and Takashi Nakanishi\*



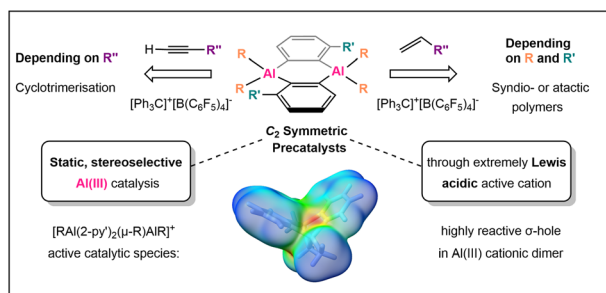
5944

### 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\*



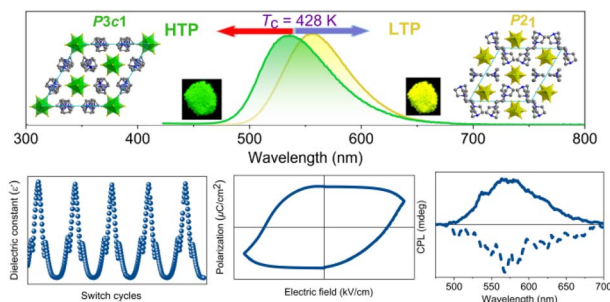
5953



### 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\*

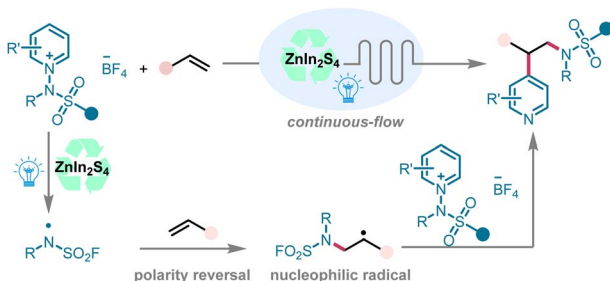
5965



### 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\*

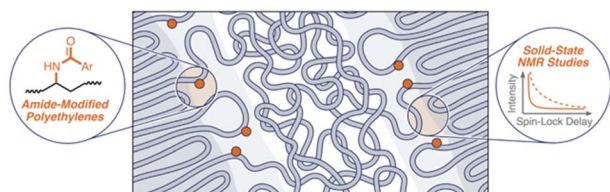
5972



### 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

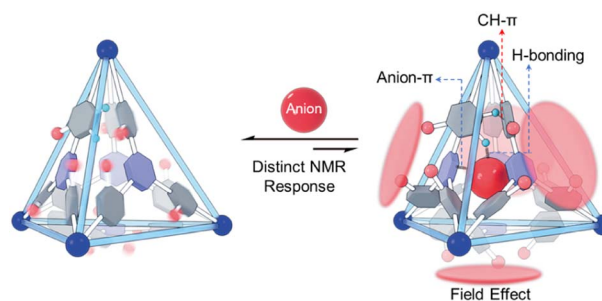
Shira Haber,\* Nicodemo R. Ciccia, Zhengxing Peng, Feipeng Yang, Julia Im, Mutian Hua, Sophia N. Fricke, Raynald Giovine, Brett A. Helms, Cheng Wang, John F. Hartwig\* and Jeffrey A. Reimer\*



5993

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

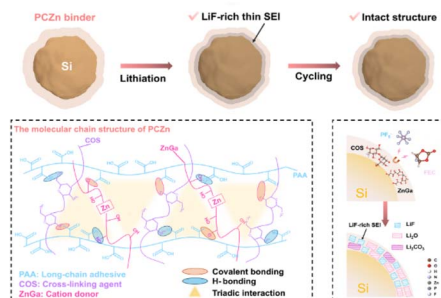
Yuyang Lu, Ping Zhou, Hua Tang, Yating Wu, Yueyan Kuang, Ze Cao, Jiyong Liu, Guangcheng Wu,\* Hongliang Chen\* and Hao Li\*



6005

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

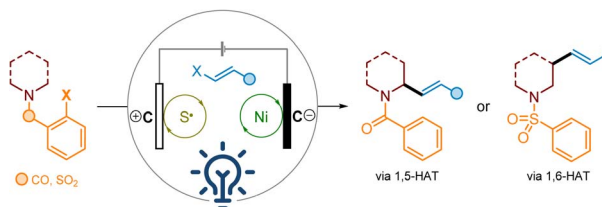
Zhipeng Wang, Qitao Shi,\* Weiqi Song, Luwen Li, Jiaqi Wang, Cheng Zhang, Alicja Bachmatiuk, Chen Lu, Peichao Zou,\* Jinho Choi,\* Yanbin Shen,\* Ruizhi Yang\* and Mark H. Rummeli\*



6017

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

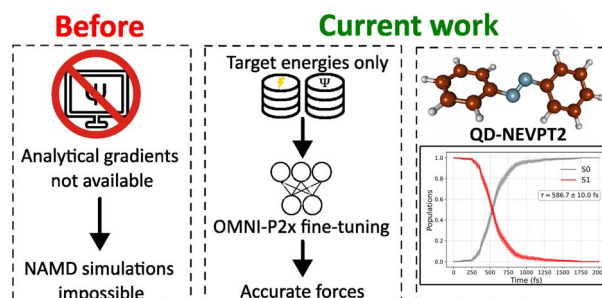
Siddharth K. Dave and Sebastian Stecko\*



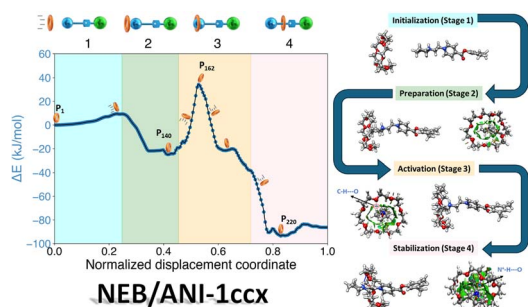
6043

### 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\*

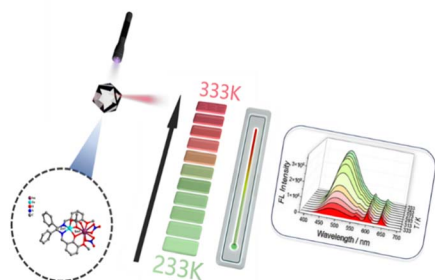
6068



### Electrostatic decatalysis through coulombic screening

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

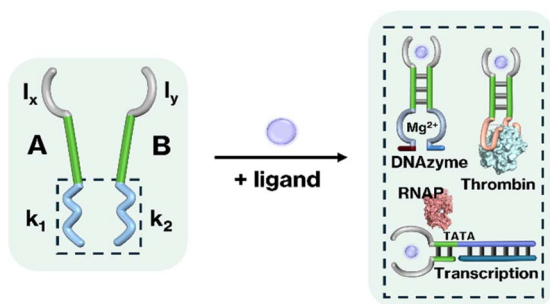
6079



### 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

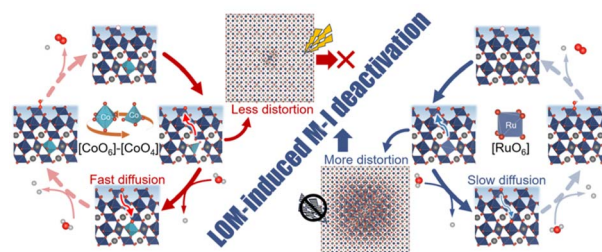
Diva Froim, Hadar Amartely, Jiantong Dong,\* Eli Pikarsky and Itamar Willner\*



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\*

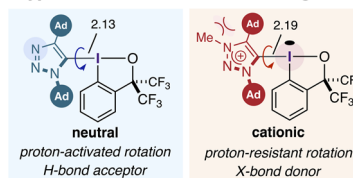


6109

### 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



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

Facile synthesis via CuAAC

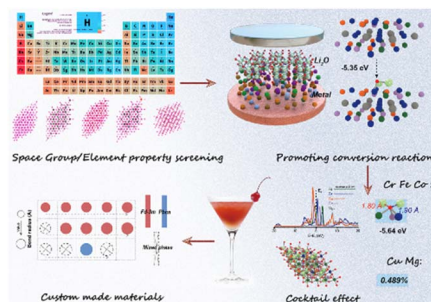
Backbone-encoded asymmetry

Divergent response & recognition

6116

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

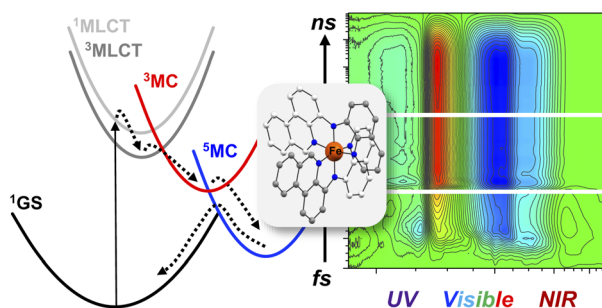
Han-Hao Liu, Jia-Lin Yang, Zhen-Yi Gu,\* Yue Liu, Xiao-Tong Wang, Chuan-Yu Zheng, Changshan Xu, Dai-Huo Liu, Wei Guo\* and Xing-Long Wu\*



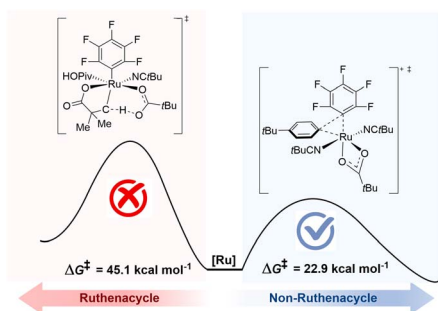
6125

### 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\*



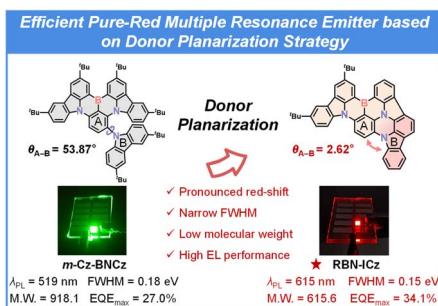
6138



### 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\*

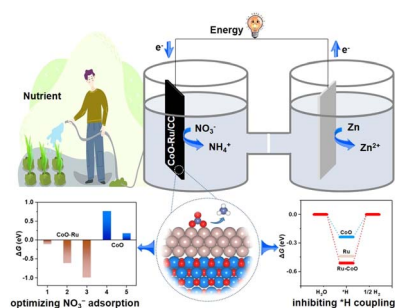
6156



### 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

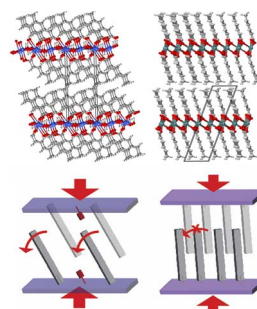
Jinxiu Zhao, Xuejing Liu, Xiang Ren,\* Dan Zhao, Zhen Li, Qing Kang, Chang-wen Zhang, Linrui Hou, Qin Wei\* and Changzhou Yuan\*



6178

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

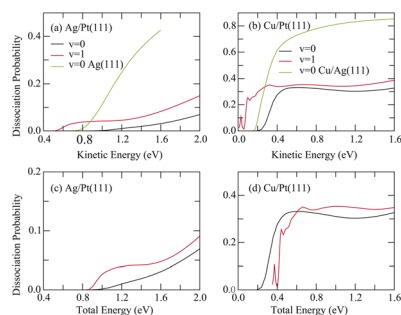
Tengteng Lyu, Jonathan B. Lefton, Martin Etter, Shrikant Bhat, Wenhao Liu, Bing Lv, Luke J. Kwan, Hao Yan\* and Tomče Runčevski\*



6187

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

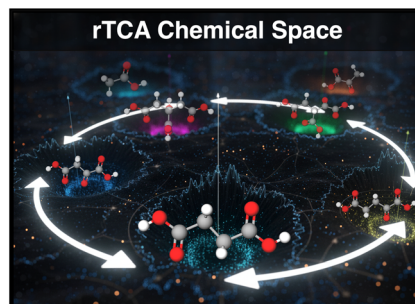
Tianhui Liu\* and Kaixin Meng



6197

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

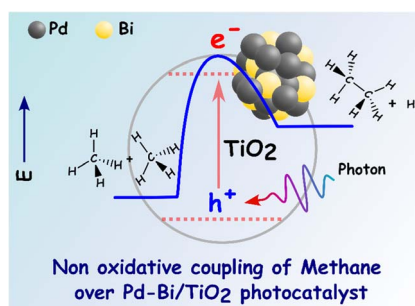
Vignesh Sathyaseelan, John Morgan\* and Brett M. Savoie\*



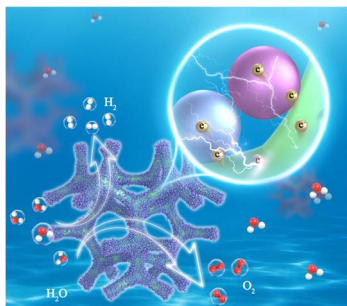
6208

### 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\*



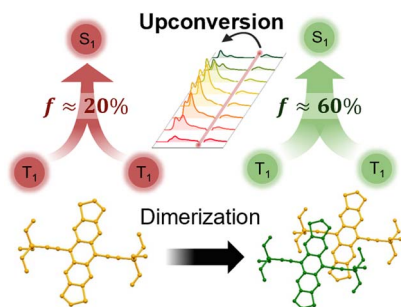
6220



### 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\*

## CORRECTIONS

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\*

