

# Chemical Science

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## IN THIS ISSUE

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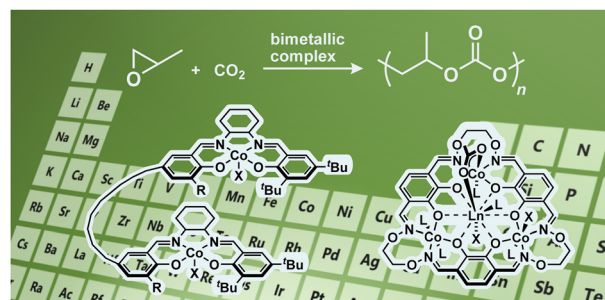
**Inside cover**  
See Joshua P. Barham, Timothy Noël *et al.*, pp. 22944–22951. Image reproduced by permission of Joshua P. Barham from *Chem. Sci.*, 2025, **16**, 22944. Acknowledgement: Image created by Sarah S. Coutts.

## COMMENTARY

22801

### A reflection on 'Bimetallic mechanism operating in the copolymerization of propylene oxide with carbon dioxide catalyzed by cobalt–salen complexes'

Koji Nakano\* and Kyoko Nozaki\*

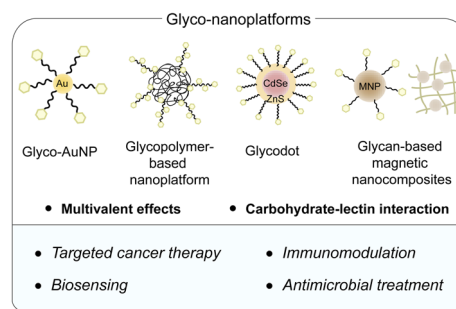


## PERSPECTIVE

22805

### Multivalently engineered glyco-nanoplatforms for targeted therapy and diagnostics

Xiao-Lin Zhang, Han Ding, Jia-Yi Zheng, Hongzhi Cao and Xue-Wei Liu\*



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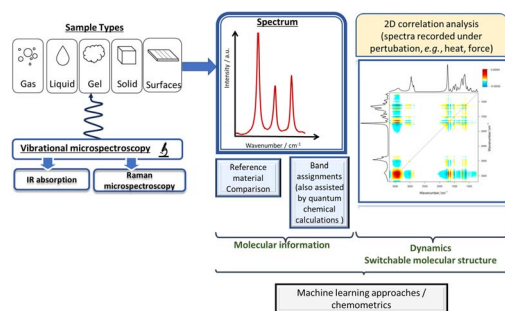
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## REVIEWS

22826

## Label-free linear and non-linear vibrational spectroscopy for functional materials: state-of-the-art and future perspectives

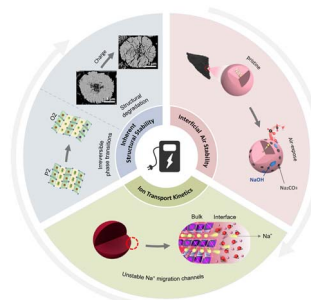
Michael Freduah Agyemang,<sup>\*</sup> Akuila L. J. L. Edwards, Stefan Zechel, Martin D. Hager, Michael Schmitt and Juergen Popp



22852

## Lattice-coherent interface-reinforced sodium-layered oxide cathodes

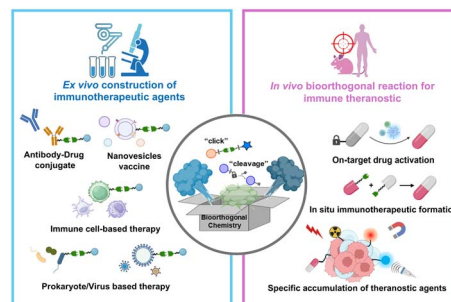
Sun-Qi Su, Qi-Cong Ling, Yan-Jiang Li,<sup>\*</sup> Ya-Ping Yan,<sup>\*</sup> Yan-Fang Zhu<sup>\*</sup> and Yao Xiao<sup>\*</sup>



22870

## A powerful bioorthogonal toolbox boosting the development of immune theranostics

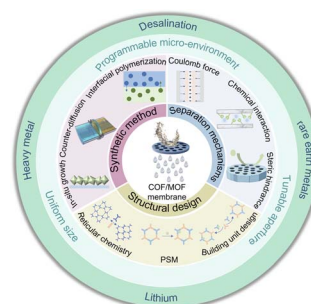
Songhan Liu, Chenyu Hua, Xianan Li, Pengcheng Yuan and Bengang Xing<sup>\*</sup>



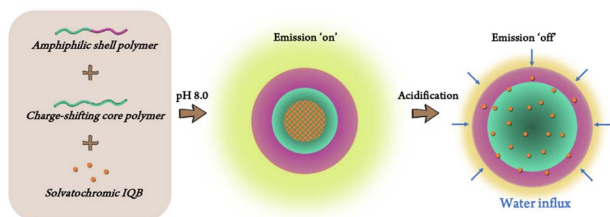
22900

## Covalent/metal-organic framework membranes with tailored pore functionality for accurate ion separation

Penglin Cheng, Tiantian Chen, Tiantian Liu, Yuhan Wei, Miaomiao Tian,<sup>\*</sup> Xueli Cao, Shi-Peng Sun, Yatao Zhang, Bart Van der Bruggen and Junyong Zhu<sup>\*</sup>



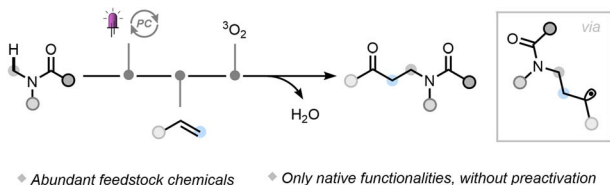
22933



### Monitoring structural change and drug release of responsive nanoparticles using polarity-sensitive fluorophores

Yanting Gao, Peter W. McDonald, Chris Ritchie\* and Georgina K. Such\*

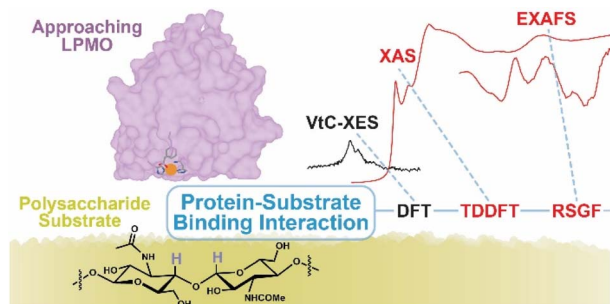
22944



### Photocatalyzed hydrogen atom transfer enables multicomponent olefin oxo-amidomethylation under aerobic conditions

Mattia Lepori, Dimitris I. Ioannou, Joshua P. Barham\* and Timothy Noël\*

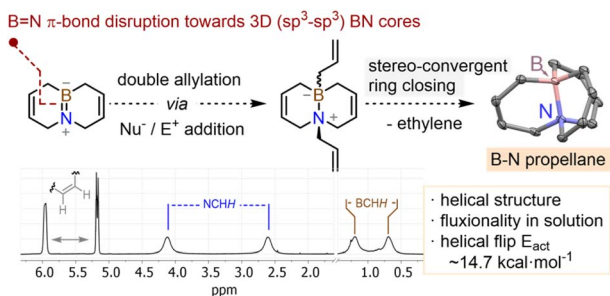
22952



### Structural and electronic modulations of lytic polysaccharide monoxygenase (LPMO) upon chitin binding: insights from X-ray spectroscopy

Chris Joseph, Ashish Tamhankar, Ole Golten, Kushal Sengupta, Sergio A. V. Jannuzzi, Morten Sørlie, Liqun Kang, Åsmund K. Røhr, Vincent G. H. Eijsink\* and Serena DeBeer\*

22970



### B–N axis as a facilitating agent for the synthesis of 3D structures: the paradigmatic case of BN-[4.4.4] propellane

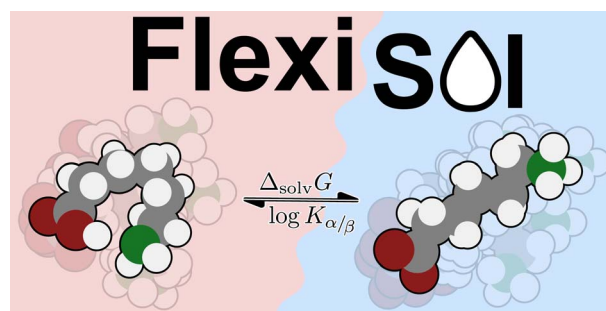
Guillem Sanz-Liarte, Josep Sauri, Pau Nolis, Ana B. Cuenca\* and Alexandr Shafir\*



22976

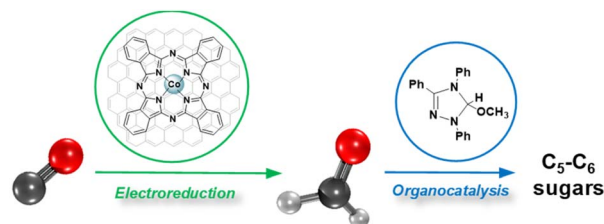
### A diverse and chemically relevant solvation model benchmark set with flexible molecules and conformer ensembles

Lukas Wittmann, Christian Erik Selzer and Stefan Grimme\*



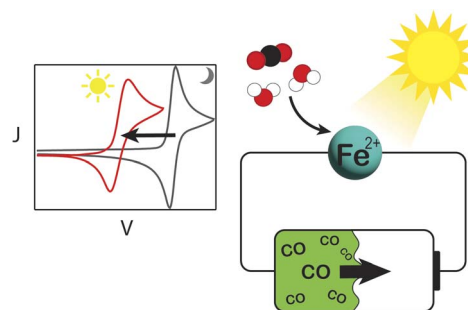
22996

### CO-to-sugars conversion from one-pot two-step electro-organocatalytic process

Ajeet Singh, David Martins-Bessa, Julien Bonin,\*  
Marc Robert\* and Sébastien Bontemps\*

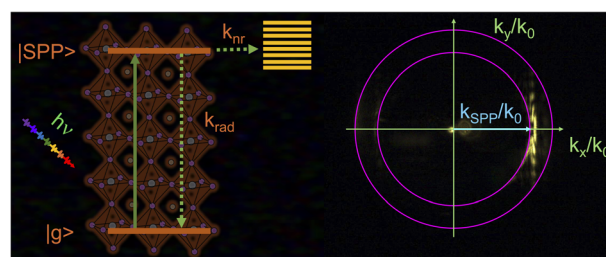
23005

### Photosynthesis of CO from CO<sub>2</sub> with an iron polypyridyl catalyst at a passivated silicon photoelectrode

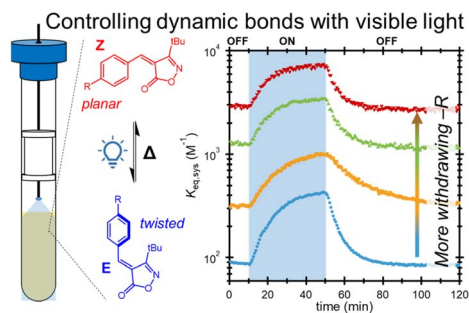
Gabiella P. Bein, Sergio Fernández, Stephen J. Tereniak,  
Renato N. Sampaio, Alexander J. M. Miller\*  
and Jillian L. Dempsey\*

23012

### Energy transfer and radiation damping in gold-MAPbI<sub>3</sub> heterostructures

Bikram Ghosh, Ajinkya Shingote, Janak Bhandari  
and Gregory V. Hartland\*

23019

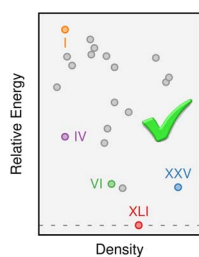


### Manipulating dynamic covalent bonds through direct photoisomerization

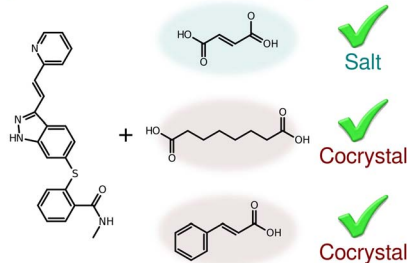
Neil D. Dolinski,<sup>\*</sup> Alex E. Crolais, Nicholas R. Boynton, Chuqiao Chen, Juan J. de Pablo, Scott A. Snyder<sup>\*</sup> and Stuart J. Rowan<sup>\*</sup>

23026

### Axitinib Neat Polymorphs



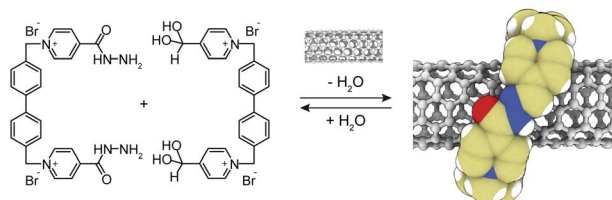
### Salts & Cocrystals



### From polymorphs to cocrystals and salts: successfully predicting axitinib's challenging crystal forms

Gregory J. O. Beran<sup>\*</sup>

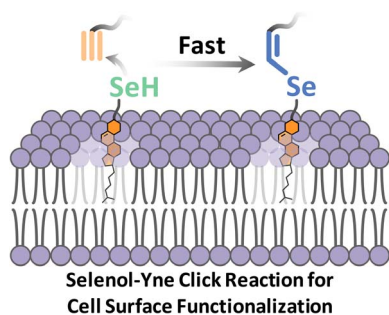
23038



### Extended white-box cyclophanes for the synthesis of mechanically interlocked derivatives of single-walled carbon nanotubes in water

Julia Villalva, Arturo Blanco-Gómez, David M. Jiménez, Alejandro López-Moreno, M. Luisa Ruiz-González, Carlos Peinador,<sup>\*</sup> Marcos D. García<sup>\*</sup> and Emilio M. Pérez<sup>\*</sup>

23047



### Efficient and rapid cell surface functionalization: a sub-minute selenol-yne click reaction for bioconjugation

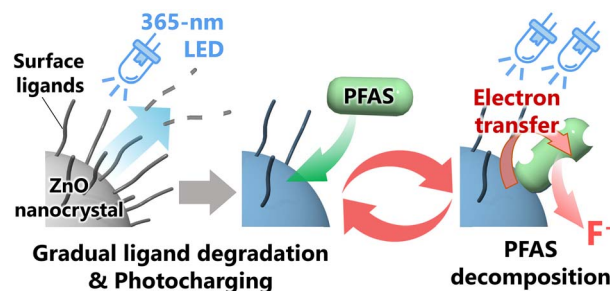
Fangjian Shan, Xingyu Heng, Lihua Yao, Guichuan Xu, Jun Hu, Xiangqiang Pan<sup>\*</sup> and Gaojian Chen<sup>\*</sup>



23055

### Photocatalytic defluorination of perfluoroalkyl substances by surface-engineered ZnO nanocrystals

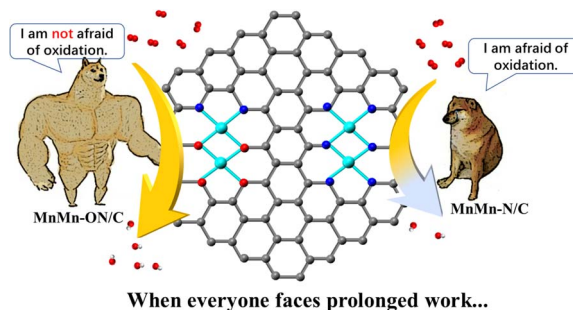
Shuhei Kanao, Mai Yamaguchi, Yuto Toyota, Yuki Nagai and Yoichi Kobayashi\*



23064

### A universal N<sub>2</sub>O<sub>4</sub>-cavity strategy for precisely spaced, durable dual-atom ORR catalysts

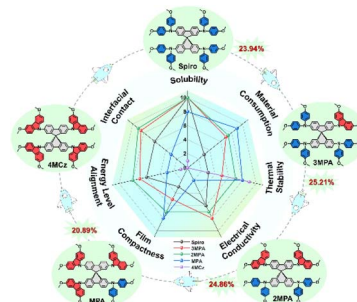
Guangxu Yao, Huijuan Zhang,\* Yangjun Luo, Chuanzhen Feng and Yu Wang\*



23077

### Rigid-flexible coupling: exquisite modulation of asymmetrical spiro-type hole-transporting materials toward efficient and stable perovskite solar cells

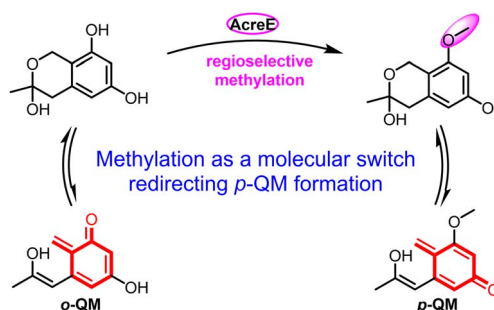
Xuran Wang, Jihong Wu, Guosen Zhang, Ruidan Zhang, Mingwei An,\* Xiaofeng He, Xiaozhen Huang, Jie Gao, Hongfang Du, Yue Wang, Dong Wei,\* Daqin Chen,\* Yang Wang\* and Wei Huang\*



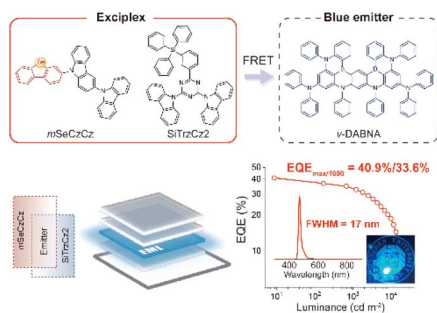
23088

### A methyltransferase molecular switch unlocks *para*-quinone methide generation and oligomerization

Chuanteng Ma, Zhenzhen Zhang, Wenxue Wang, Falei Zhang, Aowei Xie, Kaijin Zhang, Xingtao Ren, Lu Wang, Qian Che, Tianjiao Zhu, Junfeng Zhang\* and Dehai Li\*



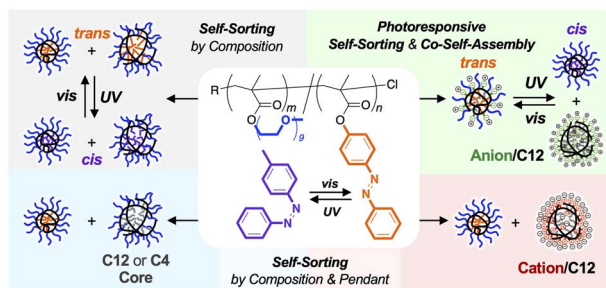
23095



### Exciplex spin-flip acceleration enables high-performance narrowband electroluminescence

Mengcheng Wang, Zhanxiang Chen,\* Manli Huang, Dengke Wang, Cheng Zhong, Zheng-Hong Lu and Chuluo Yang\*

23103

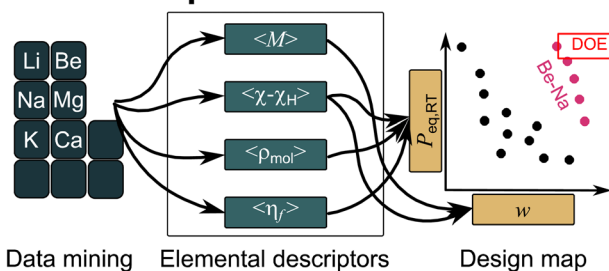


### Self-sorting systems of photoresponsive polymer micelles: isomerization drives reversible and switchable self-assembly

Rikuto Kanno, Makoto Ouchi and Takaya Terashima\*

23111

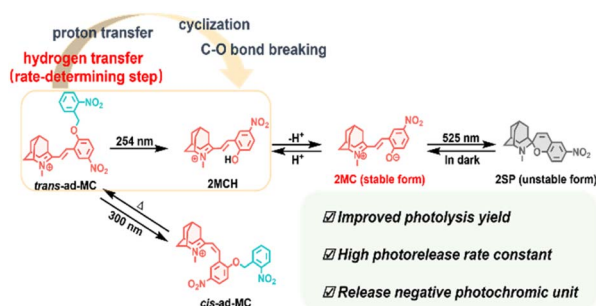
### Interpretable models



### Physically interpretable descriptors drive the materials design of metal hydrides for hydrogen storage

Seong-Hoon Jang,\* Di Zhang, Hung Ba Tran, Xue Jia, Kiyoe Konno, Ryuhei Sato, Shin-ichi Orimo\* and Hao Li\*

23121



### Tuning the photocaged spiropyran photoswitch with a sterically hindered adamantane group: releasing the stable merocyanine

Yifan Su, Xiang Li, Dexin Zheng, Joakim Andréasson, Hong Wang, Le Yu,\* Jian Chen,\* Jiani Ma\* and Yu Fang

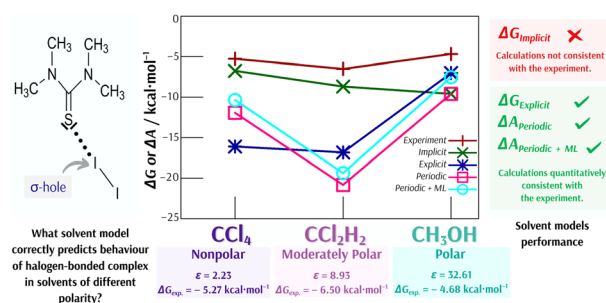
- ✓ Improved photolysis yield
- ✓ High photorelease rate constant
- ✓ Release negative photochromic unit



23129

### Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches

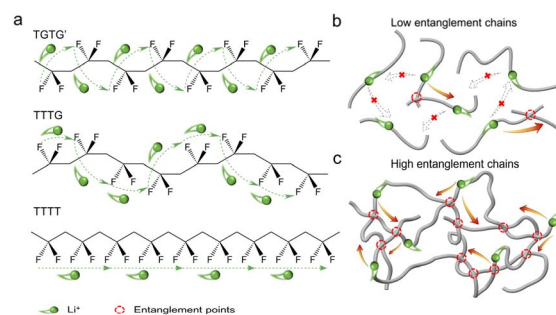
Jaroslav Vacek, Dávid Vrška, Debashree Manna,\*  
Rabindranath Lo\* and Pavel Hobza\*



23139

### Highly entangled P(VDF-TrFE) solid-state electrolytes for enhanced performance of solid-state lithium batteries

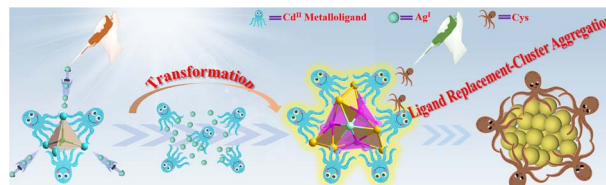
Hanghai Wu, Shuangfeng Li, Weiwei Zhu, Jie Zhang,  
Baohui Ren,\* Yan-Fei Huang\* and Zhong-Ming Li



23149

### Light-induced access to a fluorescent Cd<sub>7</sub>Ag<sub>21</sub> nanocluster from a halide-supported Cd<sub>8</sub>X nanocluster directed by a face-capping macrocyclic metalloligand

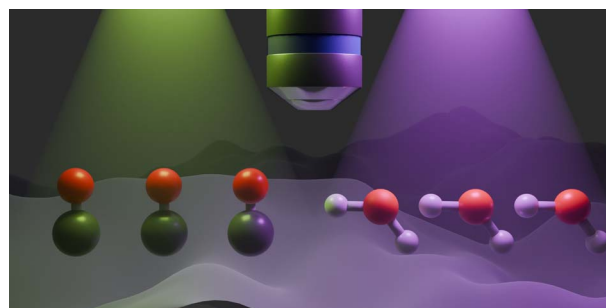
Biliu Lan, Ziling Li, Yanfang Feng, Tao Deng, Min Pan  
and Zhong Zhang\*



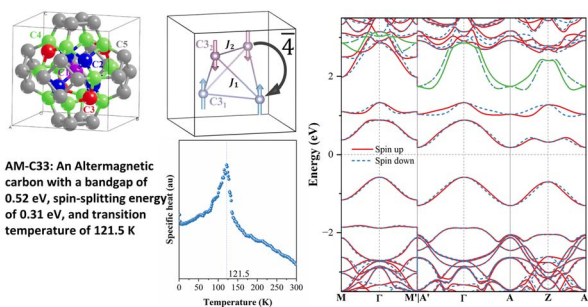
23160

### Mechanistic insights into the competition between electrochemical CO<sub>2</sub> reduction and hydrogen evolution on Ag-based electrocatalysts via operando Raman spectroscopy

Kinran Lau, Muhammad Adib Abdillah Mahbub,  
Nini Zhang, Anirudha Shekhawat, Xin Wang, Sabine Seisel,  
Ridha Zerdoumi and Wolfgang Schuhmann\*

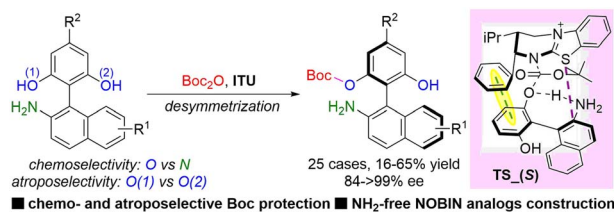


23174

**AM-C33: an altermagnetic carbon**

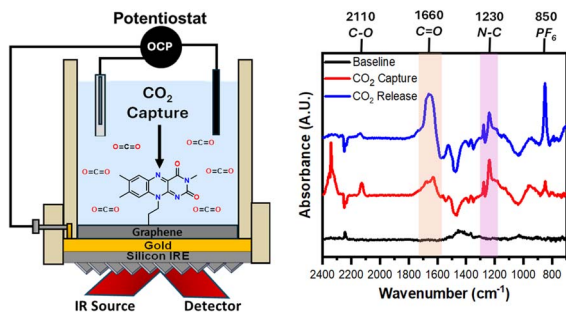
Mingqing Liao,\* Yuehua Wang, Pengcheng Ye, Chenggang Wu, Haoxin Jiang, Fei Zhou, Jintong Guan and Fengjiang Wang\*

23181

**Chemo- and atroposelective Boc protection for asymmetric synthesis of NH<sub>2</sub>-free axially chiral biaryl amino phenols**

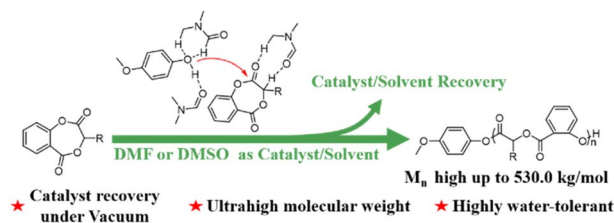
Yangyang Wang, Yike Wang, Zhe Xu, Kexin Chen, Ying-guo Liu,\* Xingkuan Chen,\* Hongwei Zhou\* and Jianfeng Xu\*

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**Real-time monitoring of the reversible capture and release of CO<sub>2</sub> on anthraquinone and riboflavin-modified graphitic electrodes using ATR-SEIRAS**

Abdur-Rahman Siddiqui, Joel Roberts, Jeanne N'Diaye, Alan L. Ferris, Kristin Martin, Seth T. Putnam, Rohit Bhargava, Jahan Dawlaty, Steven C. Zimmerman, Veronica Augustyn and Joaquín Rodríguez-López\*

23203

**DMF/DMSO-catalyzed selective ring-opening polymerization of salicylate cyclic esters**

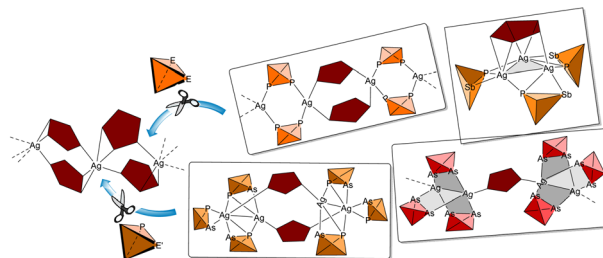
Ge Yao, Jiyu Liu, Hongjun Fu, Chunmei Wang, Guojie Li, Luya Cao, Xiaobo Pan and Jincai Wu\*



23214

## Two in one: a facile modular approach for the assembly of pnictogen-rich heteroleptic organometallic complexes

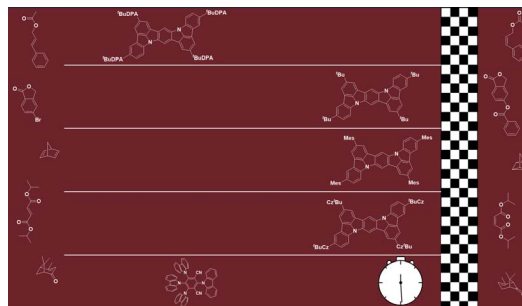
Bijan Mondal,\* Christoph Riesinger and Manfred Scheer\*



23220

## DiICz MR-TADF emitters as potent energy transfer photocatalysts

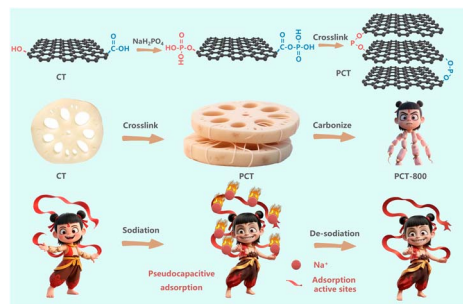
Lea Hämmerling, David Hall, Elliott Blin, Tabea Heil and Eli Zysman-Colman\*



23233

## Unraveling the origin of enhanced safety in capacitive-type carbon electrodes for 20C sodium-ion capacitors

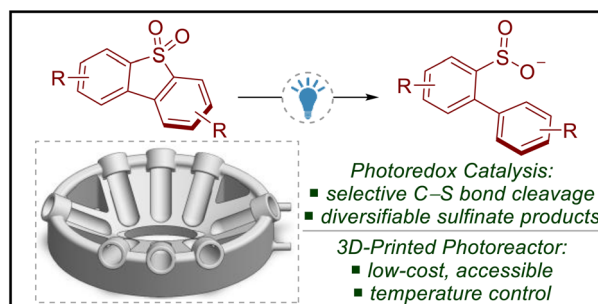
Bo Xiong, Jieming Cai, Biao Zhong, Luoming Zhang, Dongxiao Li, Jie Li, Juan Tian, Xiongwei Luo, Fei Yao, Zhiyu Zeng, Wentao Deng, Hongshuai Hou, Jialuo She,\* Tianyun Qiu,\* Guoqiang Zou,\* Dulin Yin and Xiaobo Ji



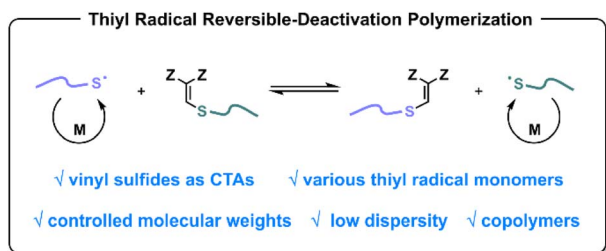
23246

## Photoredox catalysed reductive cleavage of dibenzothiophene dioxides enabled by a temperature-controlled photoreactor

Siyuan Wang, Quang Truong Le, Yoshiteru Shishido, Ismail Y. Kokculer, Ken Yamazaki, Gregory J. P. Perry,\* Adrian M. Nightingale\* and Hideki Yorimitsu\*



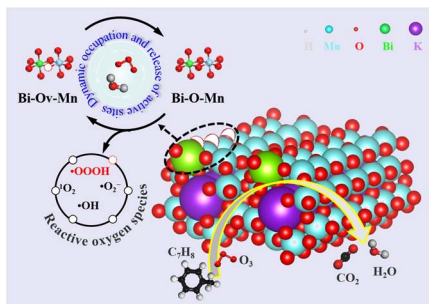
23253



### Thiyl radical reversible-deactivation polymerization *via* degenerative transfer with vinyl sulfides

Huajuan Hu, Ping Yi, Derong Cao and Hanchu Huang\*

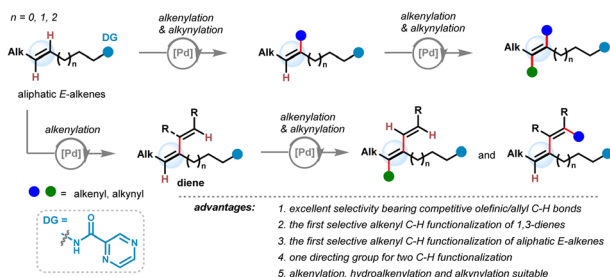
23262



### Single site of water-resistant asymmetric Bi–Ov–Mn for robust VOC ozonation at ambient temperature

Yuqin Lu, Huayang Zhang, Hua Deng,\* Jianguo Ding, Tingting Pan, Wenjie Tian, Yunbo Yu, Changbin Zhang, Wenpo Shan, Shaobin Wang, Hong He\* and Joseph S. Francisco\*

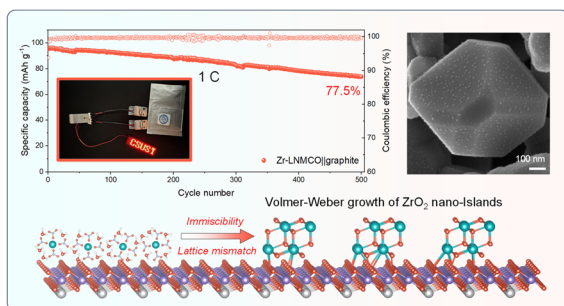
23271



### Chelation-assisted multiple and relay C–H functionalization of unactivated aliphatic *E*-alkenes

Yini Wang, Xiaoli Li, Chengxing Peng, Yu Chen, Xi Lu, Yuhang Zhu, Peiyuan Yu,\* Guofu Zhong\* and Jian Zhang\*

23282



### Volmer–Weber growth of nano-island heterostructures on spinel cathodes: a route to stable high-voltage lithium-ion batteries

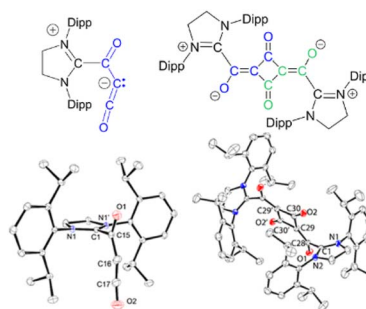
Gui Chu, Yuanqin She, Aoyu Huang, Qingquan Ye, Yimei Deng, Tongen Lin,\* Yongqi Sun, Tobias U. Schülli,\* Lianzhou Wang\* and Xiaobo Zhu\*



23292

### Trapping carbon suboxide with a carbene and isolation of the carbene-stabilized carbon suboxide dimer

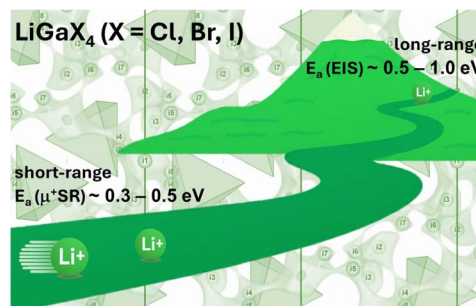
Tanner George, Erin R. Johnson and Jason D. Masuda\*



23299

### Insight into the prospects and limitations of mechanochemically-synthesised lithium tetrahalogallates, LiGaX<sub>4</sub> (X = Cl, Br, I), as Li-ion conductors

Nicolás Flores-González, Martí López, Nicolò Minafra, Jamie Jack, Jan Bohnenberger, Atsushi Inoishi, Nalin Gupta, Leandro Liborio, Francesc Viñes, Ronald I. Smith, Peter J. Baker, Ingo Krossing, Wolfgang G. Zeier, Francesc Illas and Duncan H. Gregory\*



23310

### Palladium-catalyzed amidocarbonylation of thioethers: access to α-amide-substituted thioether derivatives

Xudong Mao, Le-Cheng Wang and Xiao-Feng Wu\*



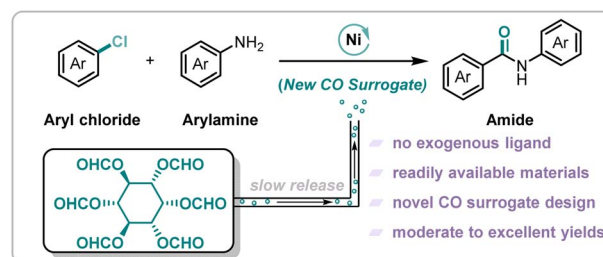
- ◆ α-C(sp<sup>3</sup>)-H functionalization
- ◆ Excellent selectivity

- ◆ 36 examples, up to 91% yield
- ◆ Broad substrate scope

23315

### Nickel-catalyzed aminocarbonylation of aryl chlorides enabled by a newly designed CO source

Zhen-Wei Liu, Yuanrui Wang, Ru-Han A. and Xiao-Feng Wu\*

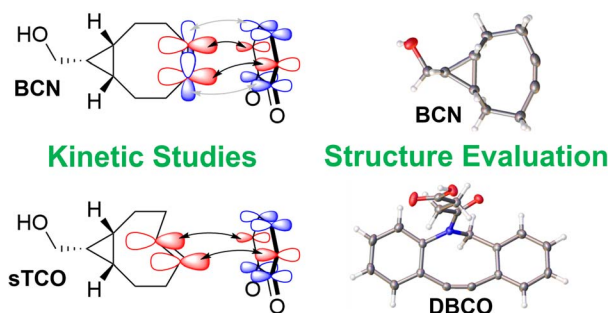




23357

### Temperature-dependent reaction rates of quinone-alkene cycloaddition reveal that only entropy determines the rate of SPOCQ reactions

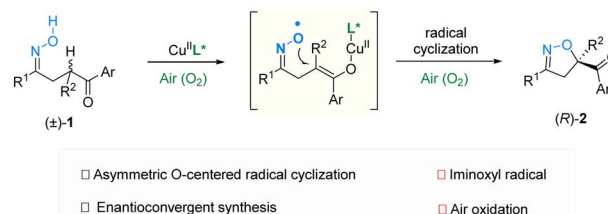
Johannes A. M. Damen, Jorge Escorihuela, Judith Firet, Han Zuilhof\* and Bauke Albada\*



23366

### Cu-catalyzed enantioconvergent oxygen-centered radical cyclization

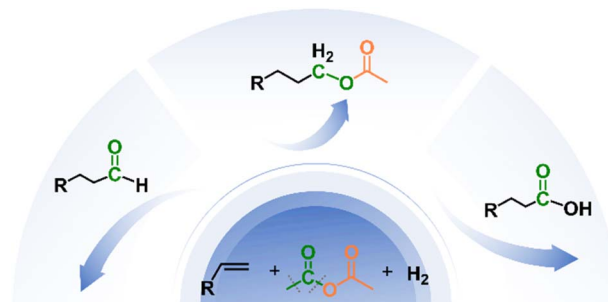
Zhen-Yu Li, Chun-Dong Huang, Chun-Yan Guan, Hui-Min Guo, Ling-Min Liu, Xiao Xiao, Beiling Gao,\* Shao-Fei Ni\* and Guang-Jian Mei\*



23376

### Acetic anhydride as a versatile carbon source in carbonylation reactions

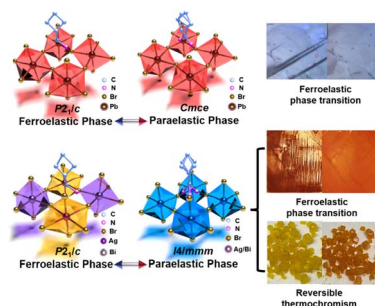
Yanru Zhang, Ying Wang,\* Junfeng Xiang, Yanyan Wang, Longbo Zhang, Jun He, Chenglong Yu, Jia Guo, Jie Cui, Xing Tong, Ziwei Zhao, Tianbin Wu, Qingli Qian\* and Buxing Han\*



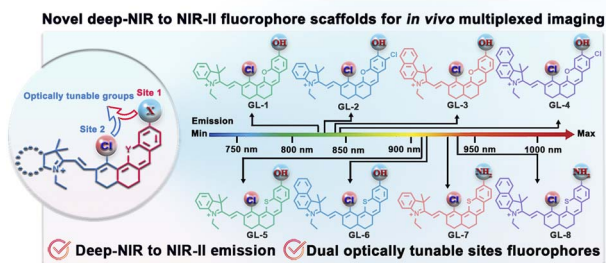
23385

### Two-dimensional lead-free double perovskite ferroelastics with dynamic thermochromism

Chang-Yuan Su,\* Heng-Guan Yi, Hao-Fei Ni, Guo-Wei Du, San-Qiang Xia, Zunqi Liu,\* Zhi-Xu Zhang\* and Da-Wei Fu\*



23394



### Deep-NIR to NIR-II hemicyanine fluorophore scaffolds with dual optically tunable sites for *in vivo* multiplexed imaging

Qinian Liu, Zhuoyang Li, Yujie Huang, Zhenni Lin, Xing-Can Shen\* and Hua Chen\*

## CORRECTIONS

23405

### Correction: Capturing and labeling CO<sub>2</sub> in a jar: mechanochemical <sup>17</sup>O-enrichment and ssNMR study of sodium and potassium (bi)carbonate salts

Austin Peach,\* Nicolas Fabregue, Célia Erre, Thomas-Xavier Métro, David Gajan, Frédéric Mentink-Vigier, Faith Scott, Julien Trébosc, Florian Voron, Nicolas Patris, Christel Gervais and Danielle Laurencin\*

23408

### Correction: Structural insights into a bacterial terpene cyclase fused with haloacid dehalogenase-like phosphatase

Keisuke Fujiyama, Hiroshi Takagi, Nhu Ngoc Quynh Vo, Naoko Morita, Toshihiko Nogawa and Shunji Takahashi\*

