

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 17(7) 3363–3860 (2026)



### Cover

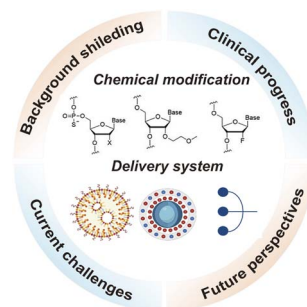
See Pedro Juan-Royo and Graeme M. Day, pp. 3480–3491. Image reproduced by permission of Paula Juan-Royo from *Chem. Sci.*, 2026, 17, 3480. Image created by Paula Juan-Royo.

## PERSPECTIVE

3377

### Navigating the next frontier in biomedicine: breakthroughs and insights in nucleic acid therapeutics

Shanchao Wu, Zihui Zhang, Zilong Zhao, Cheng Cui\* and Weihong Tan\*

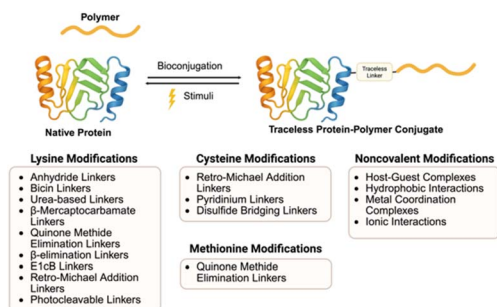


## REVIEWS

3410

### Traceless linkers used for reversible protein–polymer conjugations

Douglas A. Rose, Zihuan Fu, Mikayla F. Tan, Daniele Vinciguerra, Prieria H. Panescu and Heather D. Maynard\*



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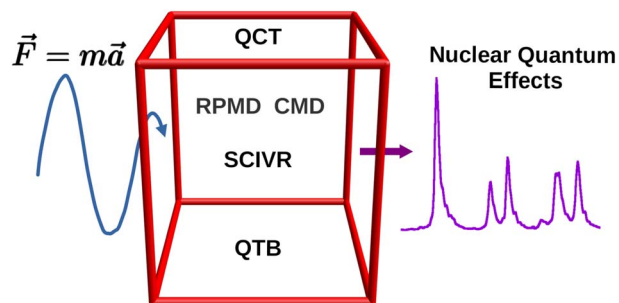
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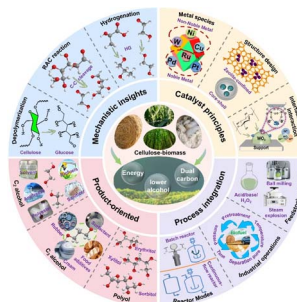
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## REVIEWS

3430

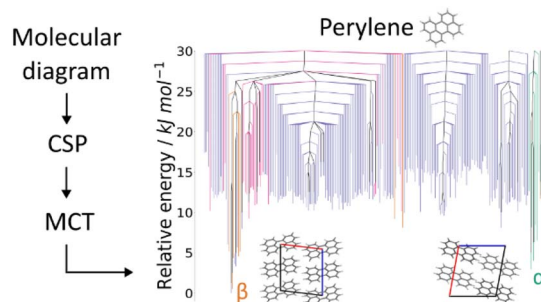
**Quantum vibrational spectroscopy with classical trajectories**Riccardo Conte,<sup>\*</sup> Chiara Aieta<sup>\*</sup> and Michele Ceotto<sup>\*</sup>

3449

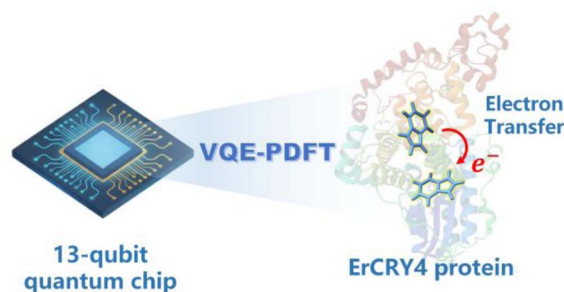
**Mechanistic insights and catalyst design for the selective hydrogenolysis of cellulose to C<sub>2</sub>-C<sub>3</sub> alcohols**Yuandong Cui, Dandan Wang, Haoxi Ben, Xiong Su,<sup>\*</sup> Xiaoli Yang<sup>\*</sup> and Yanqiang Huang

## EDGE ARTICLES

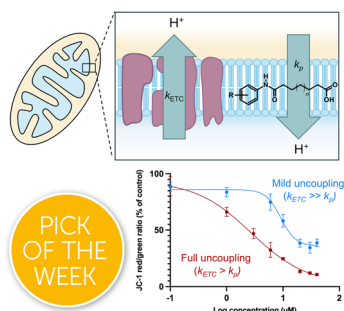
3480

**From crystal structure prediction to polymorphic behaviour: Monte Carlo threshold mapping of crystal energy landscapes**Pedro Juan-Royo and Graeme M. Day<sup>\*</sup>

3492

**Quantum-classical hybrid computation of electron transfer in a cryptochrome protein *via* VQE-PDFT and multiscale modeling**Yibo Chen, Zirui Sheng, Weitang Li, Yong Zhang, Xun Xu, Jun-Han Huang<sup>\*</sup> and Yuxiang Li<sup>\*</sup>

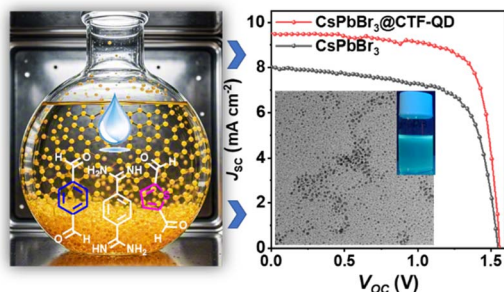
3506



### The role of transmembrane proton transport rates in mild mitochondrial uncoupling by arylamide substituted fatty acids

Ethan Pacchini, Daniel A. McNaughton, Aaron Pye, Katie A. Wilson, Philip A. Gale and Tristan Rawling\*

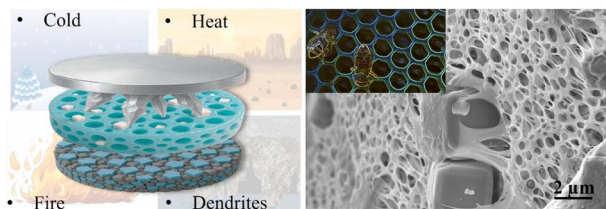
3516



### Water-mediated kinetic engineering of CTF QDs for emerging solar cells

Manying Liu,\* Zikang Lei, Peiyuan Ma, Lixin Feng, Yuanhao Wang, Dandan Zhao, Yanru Guo, Yange Zhang, Xin Zhao\* and Zhi Zheng\*

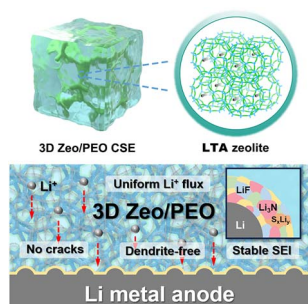
3525



### Robust Janus-faced quasi-solid-state honeycomb-mimicking electrolytes for the fast transport and adequate supply of sodium ions

Fang Chen, Yadan Xie, Zhoubin Yu, Na Li, Yu Qiao\* and Xiang Ding\*

3533



### A solid composite electrolyte based on three-dimensional structured zeolite networks for high-performance solid-state lithium metal batteries

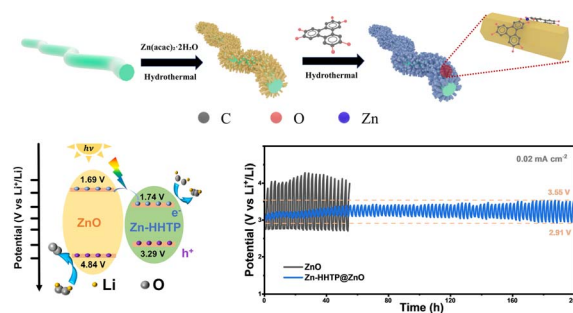
Zhaodi Luo, Yuxin Cui, Zixuan Zhang, Malin Li\* and Jihong Yu\*



3544

## Designing wide-spectrum-responsive cathode catalysts with abundant active sites for high-performance photo-enabled lithium–oxygen batteries *via* band engineering

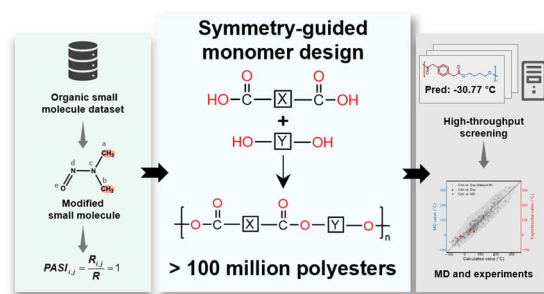
Yanhui Gan, Min Yue, Yujia Niu, Chengjie Wu, Songtao Zhang, Mengtao Ma, Hao Gong,\* Hairong Xue\* and Renzhi Ma\*



3553

## Symmetry-guided monomer design enables the combinatorial synthesis and targeted screening of polyesters

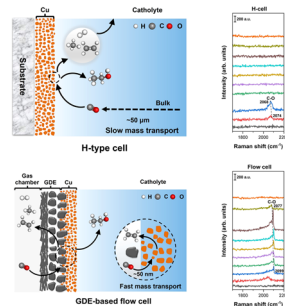
Xiaojie Feng, Xiaoying He, Jiayi Zhu, Li-Hong Lin, Qiaoyan Shang, Zheng-Hong Luo, Yin-Ning Zhou\* and Fangyou Yan\*



3563

## Mass transport-dependent *in situ* Raman detection in CO/CO<sub>2</sub> electrolysis

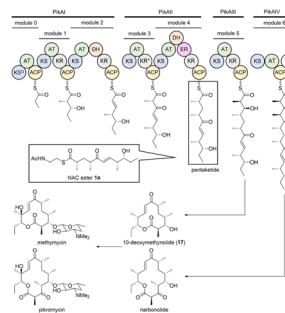
Wen Yan, Hangyu Bu, Xinjuan Du, Beining Xu, Jia Liu\* and Ming Ma\*



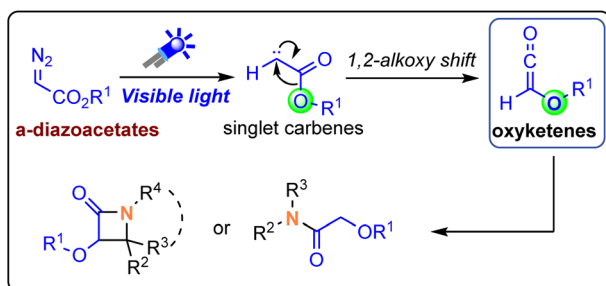
3572

## Characterization of the ketoreductase domain of pikromycin module 2

Eiji Okamura, Kosuke Ohsawa, Hidetoshi Ban, Yoshiyuki Sugiyama, Junko Hashimoto, Kei Kudo, Masahito Yoshida, Kazuo Shin-ya, Haruo Ikeda, Shunji Takahashi\* and Takayuki Doi\*



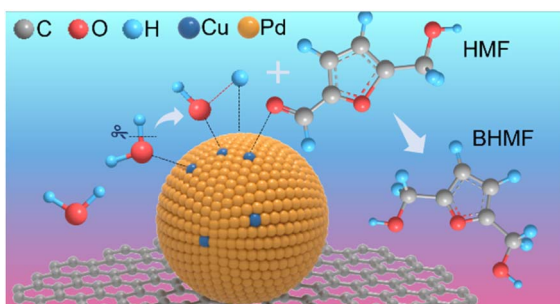
3587



### Visible light-induced 1,2-alkoxy shift of $\alpha$ -diazoacetates for Wolff rearrangements – access to oxyketenes

Yang Liu, Zi-Yi Xie, Lennard Kloene, Cong-Lun Xu, Jian-Peng Tai, Yu Zhu, Bao-Gui Cai, Chongqing Pan,\*  
Rene M. Koenigs\* and Jun Xuan\*

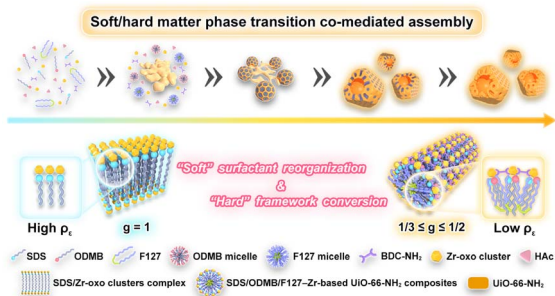
3593



### Pd–Cu dual-site tuned H adsorption for efficient electrocatalytic hydrogenation of HMF

Guozhou Feng, Yuxin Fan, Lechen Diao,\* Zhichao Miao and Jin Zhou\*

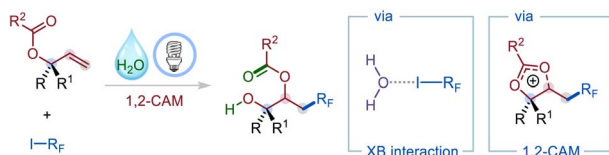
3605



### Biomimetic cooperative assembly for tailoring anisotropic hierarchically porous metal-organic frameworks

Ruigang Sun, Ji Han, Bin Zhao, Bohan Liu, Guangrui Chen, Haidong Xu, Baiqi Wang, Yanjing Gao, Song Lin Zhang, Yusuke Yamauchi, Xiaoxin Chen\* and Buyuan Guan\*

3618



### Halogen bonding-induced 1,3-carbohydroxylation of allyl carboxylates via 1,2-cationic acyloxy migration (1,2-CAM)

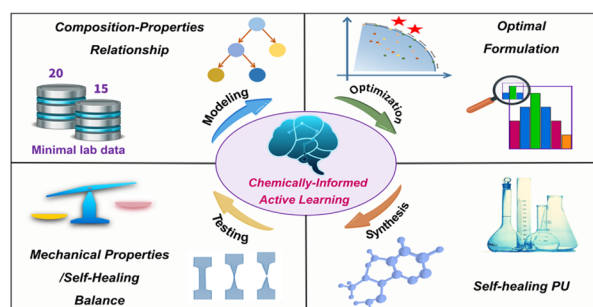
Sahil Sharma, Gaoyuan Zhao, Loay Bedda, Arman Khosravi, Djamaladdin G. Musaev and Ming-Yu Ngai\*



3627

### Chemically-informed active learning enables data-efficient multi-objective optimization of self-healing polyurethanes

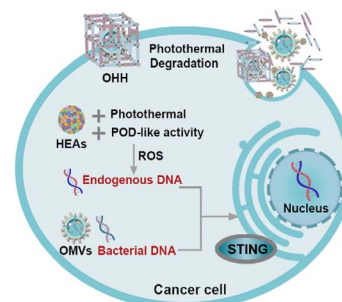
Kang Liang, Xinke Qi, Xu Xiao, Li Wang\* and Jinglai Zhang\*



3639

### In situ released bacterial membrane vesicles activate the STING pathway via boosting the intracellular DNA pool for immunotherapy

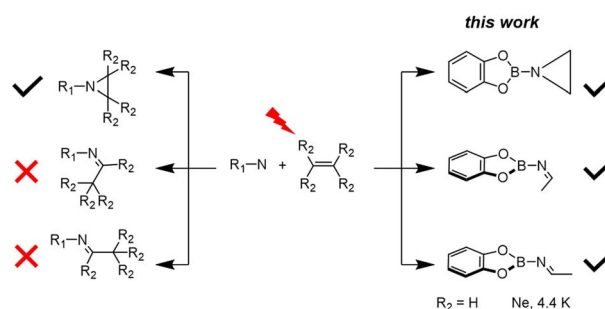
Wenjie Wang, Anjun Song, Fang Pu, Yanjie Zhang, Jinsong Ren\* and Xiaogang Qu\*



3651

### Unusual nitrene reactivity: imine formation in the photochemical reaction of a borylnitrene with ethene

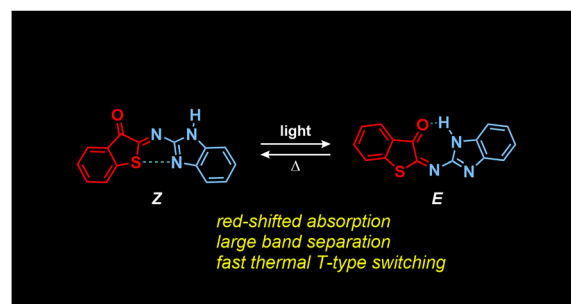
Virinder Bhagat and Holger F. Bettinger\*



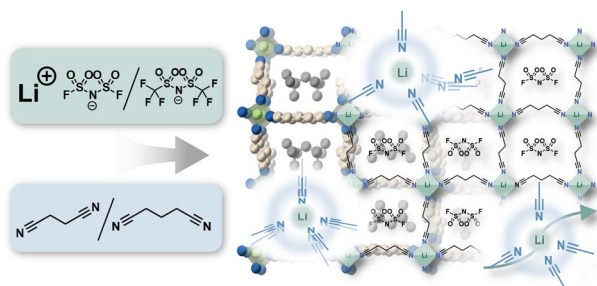
3658

### Heteroaryl iminothioindoxyl (HA-ITI) photoswitches via regioselective aza-Wittig synthesis: unifying red-shifted absorption, large E/Z band separation, and tunable thermal recovery

Jialei Chen-Wu, Carlos Benitez-Martin,\* José A. González-Delgado, Flip de Jong, Eduard Fron, Gert Steurs, Antonio J. Martínez-Martínez, Francisco Nájera, Morten Grøtli,\* Johan Hofkens,\* Joakim Andréasson\* and Uwe Pischel\*



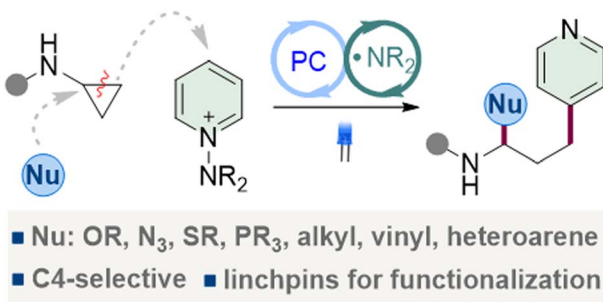
3669



### Soft crystalline properties of 2D frameworks constructed from lithium ions and dinitriles

Taichi Nishiguchi, Kotoha Kageyama, Takuya Kurihara, Nanae Shimanaka, Shun Tokuda, Shuto Tsuda, Nattapol Ma and Satoshi Horike\*

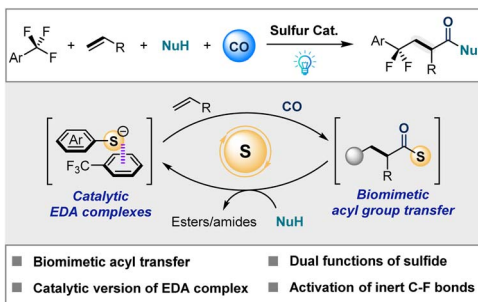
3675



### Photocatalytic construction of *N*-acyl-*N,O*-acetal-linked pyridines via aminocyclopropane ring opening

Doyoung Kim, Eunseon Yang, Yoonhee Cho and Sungwoo Hong\*

3683

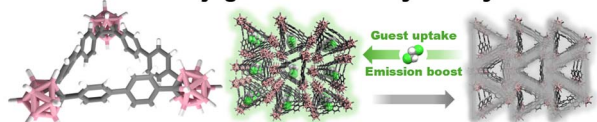


### Biomimetic sulfur-catalyzed carbonyl transfer enables the carbonylative difunctionalization of unactivated alkenes

Yuanrui Wang and Xiao-Feng Wu\*

3691

### Porous Conjugated Carboracycle Crystal



### Guest-induced emission enhancement in the permanent porous conjugated carboracycle crystal

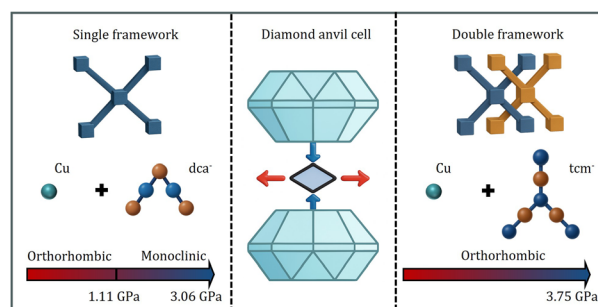
Kazuhiro Yuhara, Sota Takemori, Takumi Yanagihara, Shunsuke Ohtani, Tomoki Ogoshi and Kazuo Tanaka\*



3700

### Negative and zero linear compressibility in copper dicyanamide and tricyanomethanide

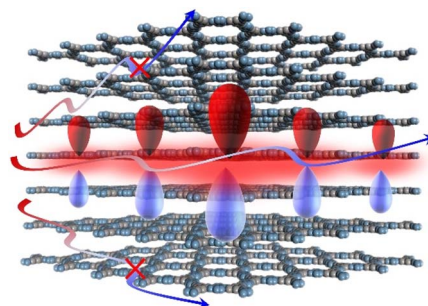
Muzi Chen,<sup>\*</sup> Hanna L. B. Boström, Dominik Daisenberger, Nicholas P. Funnell, Christopher J. Ridley and Andrew B. Cairns<sup>\*</sup>



3708

### Unveiling the electron–phonon coupling anisotropy in 2D covalent organic frameworks

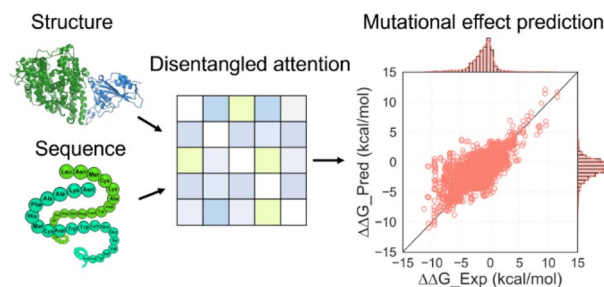
Yilin Zhang, Zhixiang Dai, Zihan Tan, Hongli Yang, Chao Xu, Shengyang Zhou<sup>\*</sup> and Zhong-Ming Li



3719

### DSSA-PPI: enhancing binding affinity change prediction upon protein mutations using disentangled structure–sequence aware attention

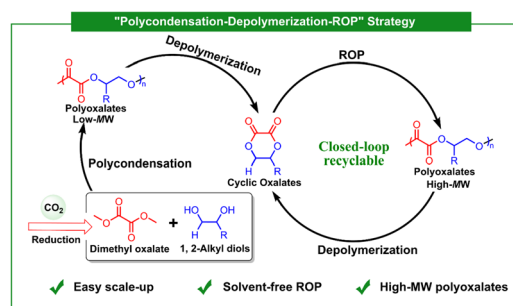
Juhong Wu, Jiehui Sun, Tian Liang, Yongqi Zhang, Han Zhang, Tianyi Zhang, Xianmin Feng, Ping Gao, Peng Xu<sup>\*</sup> and Jinyu Li<sup>\*</sup>



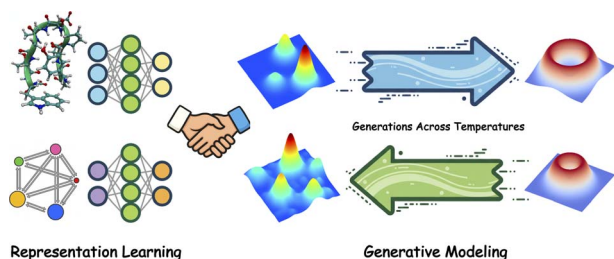
3733

### A Polycondensation–depolymerization strategy enables closed-loop recyclable polyoxalates via ring-opening polymerization of six-membered cyclic oxalates

Yalei Liu, Zheng Li, Dongfang Zhao, Yong Shen<sup>\*</sup> and Zhibo Li<sup>\*</sup>



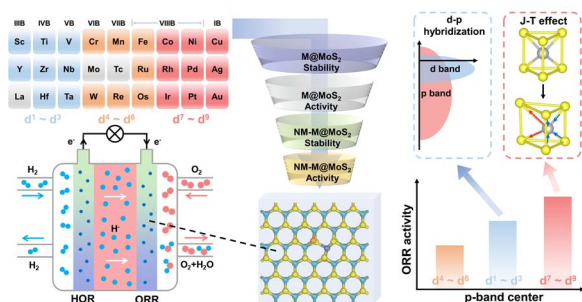
3743



### Latent thermodynamic flows: unified representation learning and generative modeling of temperature-dependent behaviors from limited data

Yunrui Qiu, Richard John, Lukas Herron and Pratyush Tiwary\*

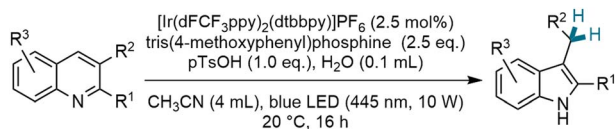
3758



### New theoretical insights into doping-induced enhancement of ORR activity in molybdenum disulfide: d–p hybridization or the Jahn–Teller effect?

Jia-Cheng Chen, Mao-Jun Pei, Wen-Bei Yu, Xiang Gao, Qing Zeng, Jia-Ming Xu, Wei Yan, Yao Liu,\* Guo-Qiang Luo\* and Jiujun Zhang\*

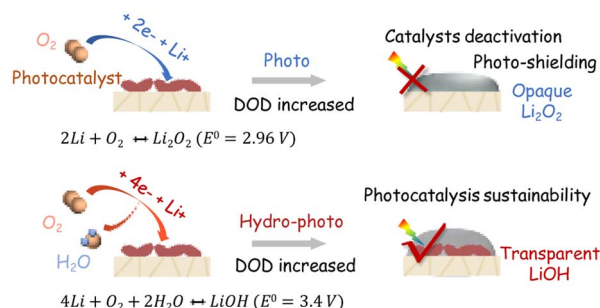
3775



### Reductive rearrangement of substituted quinolines to 2,3-disubstituted indoles enabled by water activation

Nico Spreckelmeyer, Jieun Kim, Jessika Lammert, Elena Sophia Horst, Jingjing Zhang and Armido Studer\*

3783



### Hydro-photo-synergy unlocks deep and reversible chemistry of solid-state lithium–oxygen batteries

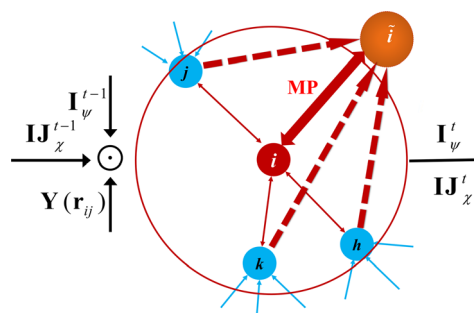
Sijia Chi, Zhenshen Li, Xunjie Yin, Shuoyi Chen, Xuerui Yi, Yiqiao Wang, Yong Guo, Fangbing Li, Shichao Wu\* and Quan-Hong Yang\*



3793

### Node-equivariant message passing for efficient and accurate machine learning interatomic potentials

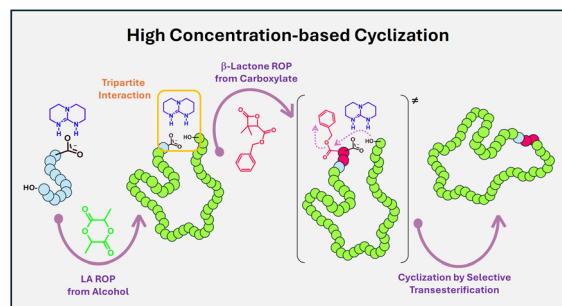
Yaolong Zhang\* and Hua Guo



3804

### Tripartite hydrogen-bonding as a driving force for high-concentration cyclization of poly(L-lactide)

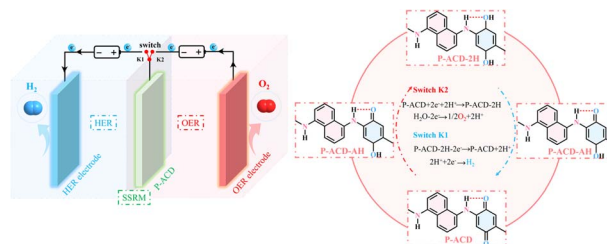
Sébastien Moins, Alexandre Mignot, Céline Henoumont, Sophie Laurent, Philippe Leclère and Olivier Coulembier\*



3810

### Membrane-free two-step water electrolysis enabled by a stable organic redox mediator

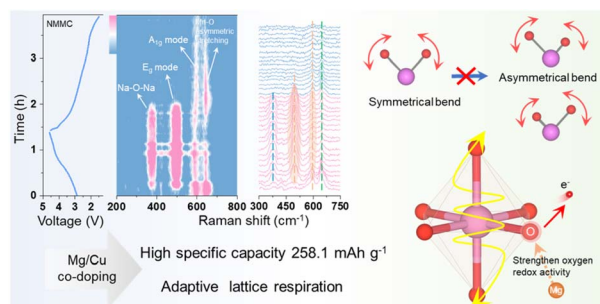
Xiao Liu, Jinlan Tang, Duan Bin,\* Qiang Huang, Congcong Li, Linyan Su, Wei Qin, Yu Ge, Xingru Chen, Hongbin Lu, BeiBei Yang\* and Yonggang Wang\*



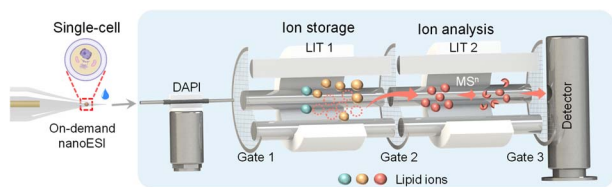
3819

### Adaptive lattice breathing enabled by Cu/Mg co-doping for stable anionic redox chemistry in sodium layered oxides

Ziqin Zhang, Wenji Yin, Jiming Peng,\* Fenghua Zheng, Qichang Pan, Hongqiang Wang,\* Qingyu Li and Sijiang Hu\*



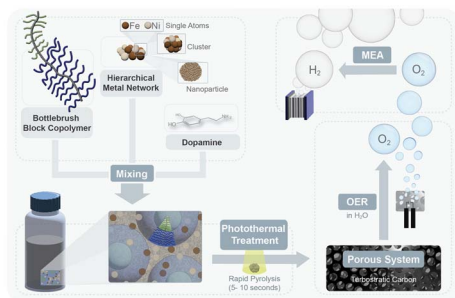
3828



### Single-cell structural lipidomics using a miniature dual-LIT mass spectrometer

Zhijun Cai, Ningxi Li, Simin Cheng, Zheng Ouyang\* and Xiaoxiao Ma\*

3841



### Alkaline electrocatalytic water oxidation by Fe–Ni nanostructures on porous turbostratic carbon with tailorable metal–metal active sites

Dipankar Saha, Chaoyun Tang, Javed Khan, Pulkit Jain, Cheng-Jie Yang, Chung-Li Dong, Richard F. Webster, Chi-Liang Chen, Zhu Chen, Peng Bai, Richard M. Tilley, Nianqiang Wu\* and James J. Watkins\*

## CORRECTIONS

3857

### Correction: Chemically-informed active learning enables data-efficient multi-objective optimization of self-healing polyurethanes

Kang Liang, Xinke Qi, Xu Xiao, Li Wang\* and Jinglai Zhang\*

3858

### Correction: Stapled histone H3 tails are super-substrates for lysine methyltransferase SETD7

Nurgül Bilgin, Laust Moesgaard, Jacob Kongsted and Jasmin Mecinović\*

