

# Journal of Materials Chemistry A

Materials for energy and sustainability

[rsc.li/materials-a](https://rsc.li/materials-a)

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.

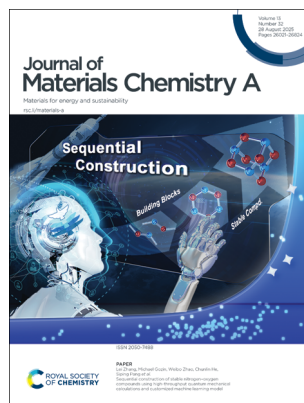
## IN THIS ISSUE

ISSN 2050-7488 CODEN JMCAET 13(32) 26021–26824 (2025)



### Cover

See Christina Schenk, De-Yi Wang *et al.*, pp. 26228–26243. Image reproduced by permission of Christina Schenk, Jose Hobson, Maciej Haranczyk and De-Yi Wang from *J. Mater. Chem. A*, 2025, 13, 26228.



### Inside cover

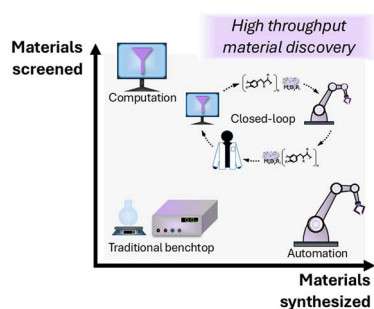
See Lei Zhang, Michael Gozin, Weibo Zhao, Chunlin He, Siping Pang *et al.*, pp. 26244–26254. Image reproduced by permission of Lei Zhang from *J. Mater. Chem. A*, 2025, 13, 26244.

## REVIEWS

26041

### High throughput computational and experimental methods for accelerated electrochemical materials discovery

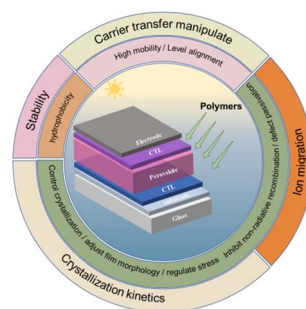
Uzoma Nwabara, Kunran Yang, Akshay Talekar, Varinia Bernales, Jorge González, Stuart Miller\* and Jinfeng Wu\*



26067

### Polymers for perovskite solar cells: advances and perspectives

Zhiwei Chen, Zhichao Lin,\* Yibing Wu and Xinhua Ouyang\*



**GOLD  
OPEN  
ACCESS**

# EES Solar

**Exceptional research on solar  
energy and photovoltaics**

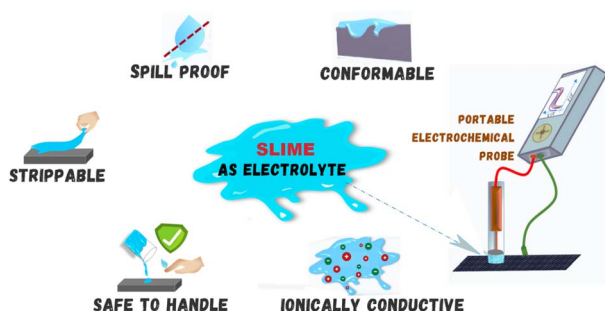
Part of the EES family

**Join  
in** | Publish with us  
[rsc.li/EESolar](https://rsc.li/EESolar)



## PERSPECTIVES

26202

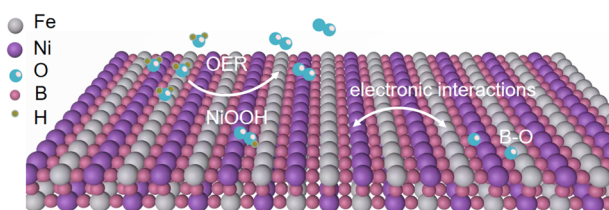


## Repurposing PVA-based slime to address electrolyte challenges in portable electrochemical devices

Anu Renjith, V. Lakshminarayanan and Harish C. Barshilia\*

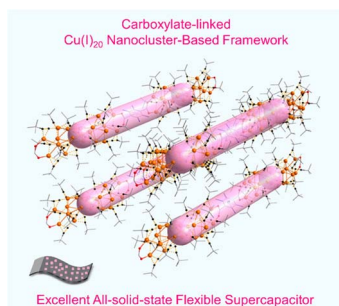
## COMMUNICATIONS

26215

*In situ* borate generation by amorphous Ni–Fe–B nanosheets: a highly active electrocatalyst for oxygen generation in alkaline seawater

Li He,\* Zhengwei Cai and Chaolin Wang\*

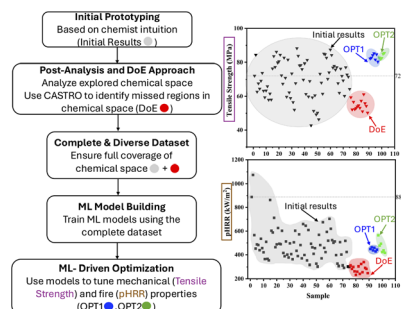
26223

A carboxylate-linked atomically precise one-dimensional Cu<sub>20</sub> nanocluster-based framework for all-solid-state flexible supercapacitors

Wenqing Wang, Yang Wang\* and Wai-Yeung Wong\*

## PAPERS

26228



## Data-driven design and green preparation of bio-based flame retardant polyamide composites

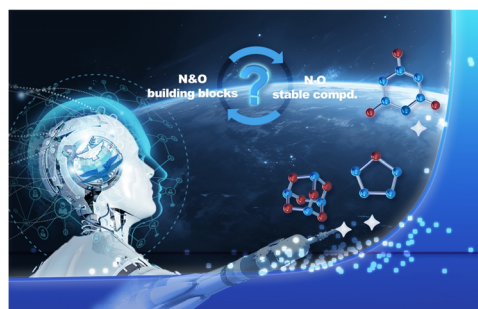
Christina Schenk,\* Jose Hobson, Maciej Haranczyk and De-Yi Wang\*



26244

### Sequential construction of stable nitrogen–oxygen compounds using high-throughput quantum mechanical calculations and customized machine learning model

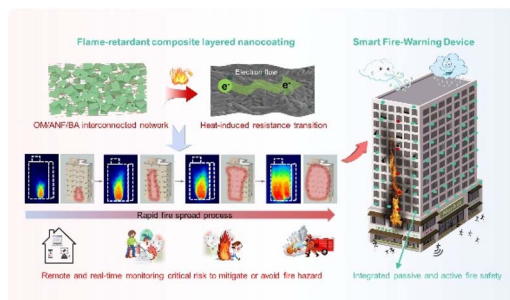
Chenyue Wang, Lei Zhang,\* Chuanyue Chen, Kaile Dou, Jinya Zhang, Chongyang Li, Michael Gozin,\* Weibo Zhao,\* Chunlin He\* and Siping Pang\*



26255

### Thermally induced cyclic resistance transition of a transparent and flame-retardant layered oxidized MXene composite nanocoating for remote-synch fire monitoring

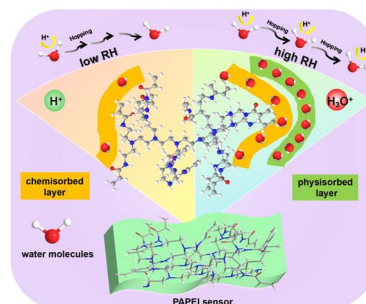
Ye-Jun Wang, Bi-Fan Guo, Ling-Yu Lv, Cheng-Fei Cao,\* Pei-Yuan Lv, Yang Li, Guo-Dong Zhang, Jie-Feng Gao, Pingan Song, Kun Cao and Long-Cheng Tang\*



26268

### A flexible polyethyleneimine film sensor for high humidity monitoring

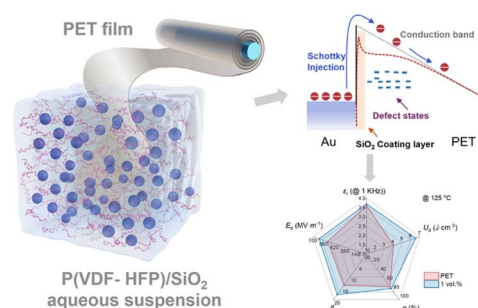
Xiaosai Hu, Haoran Cao, Haoqi Liu, Hongming Lv, Yuanyu Ge\* and Tianchi Zhou\*



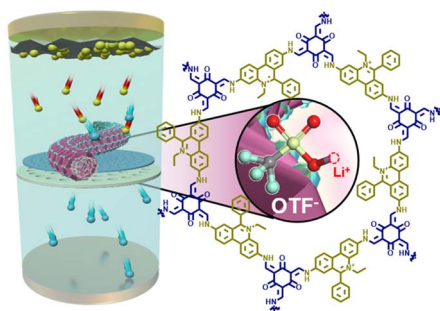
26279

### A simple surface engineering approach to enhance the Schottky barrier of polymer dielectrics for superior energy storage performance

Tao Liu, Yang Liu, Jin Qian, Jijia Ren, Jiwei Zhai,\* Tao Zhou,\* Yao Zhou, Gui-Wei Yan, Di-Ming Xu, Wenfeng Liu\* and Di Zhou\*



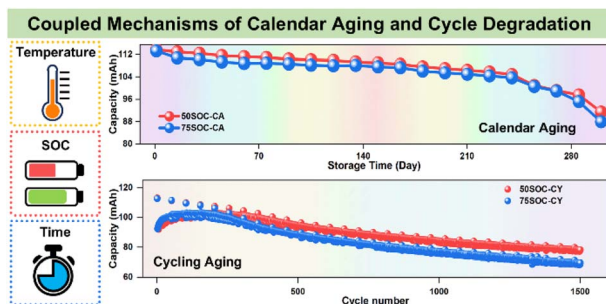
26288



### Regulating the anionic environment of the COF@CNT composite for kinetics-boosted and wide-temperature lithium–sulfur batteries

Zhangyu Zheng, Wancheng Zhang, Qingyu Dai, Huishu Wu,\* Zhiwei Huang, Yuning Zhang,\* Bo Peng, Lianbo Ma and Jie Xu\*

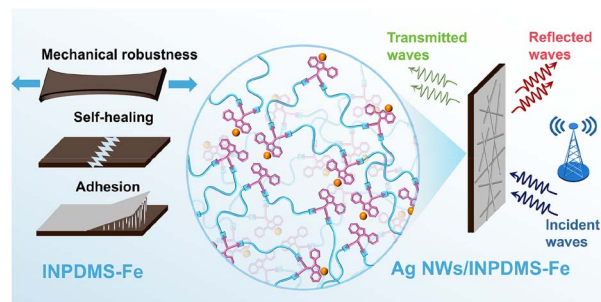
26297



### Coupled influence of state-of-charge and storage temperature on calendar aging and subsequent cycle degradation in LiFePO<sub>4</sub>/graphite pouch cells

Wenjun Shen, Jinyang Dong,\* Yun Lu, Kang Yan, Yibiao Guan,\* Guangjin Zhao, Bowen Li, Xi Wang, Rui Tang, Jialong Zhou, Ning Li, Yuefeng Su,\* Feng Wu and Lai Chen\*

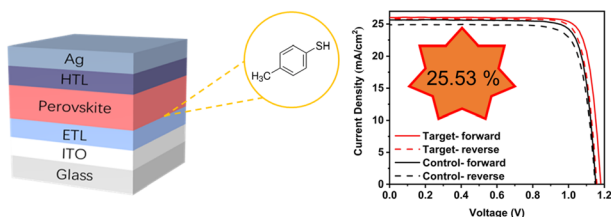
26310



### A room-temperature self-healing and mechanically robust siloxane elastomer *via* synergistic complexation and cation– $\pi$ interactions for high-performance electromagnetic interference shielding

Suting Chen, Ziyi Liu, Tian Qiu, Ting Zhang, Chaoqun Ma, Dongjin Xie, Tengning Ma, Li Yang, Guanjun Chang\* and Ying Huang\*

26320



### Synergistic engineering of buried interfaces for high-efficiency and stable perovskite solar cells

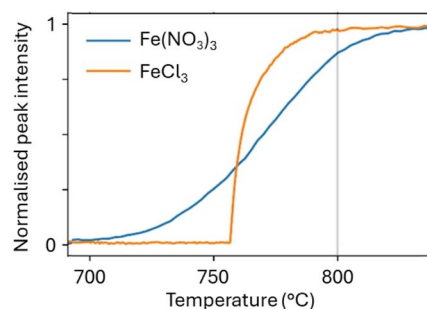
Yikun Hua, Xinyue Song, Lei Zhao, Chao Wu, Jie Zhang, Weiyuan Chen and Lin Song\*



26327

### *In situ* TEM and synchrotron SAXS/WAXS study on the impact of different iron salts on iron-catalysed graphitization of cellulose

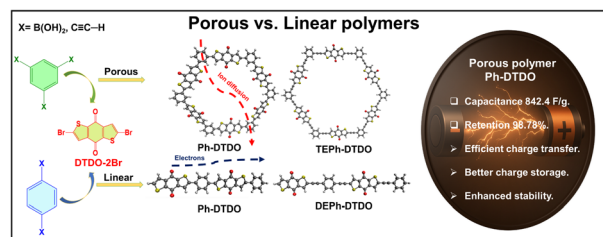
Emily C. Hayward, Masaki Takeguchi, Harry J. Lloyd, Joshua M. Stratford, Andrew J. Smith, Tim Snow, Joaquin Ramirez-Rico and Zoe Schnepf\*



26337

### Engineering redox-active benzo[1,2-*b*:4,5-*b'*] dithiophene-based conjugated polymers: tuning porosity and linker architecture for high-performance supercapacitors

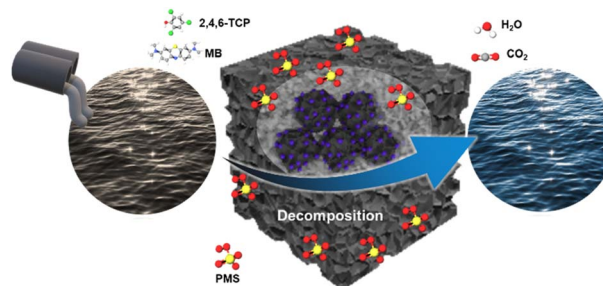
Yousra M. Nabil, Shimaa Abdelnaser, Ahmed A. K. Mohammed, Shiao-Wei Kuo and Ahmed F. M. EL-Mahdy\*



26350

### Facile fabrication of MOF and natural polymer-derived carbon-aerogels with multiscale porosity for persulfate activation in water treatment

Minsoo Yoon, Hyunuk Jeon, Jisoo Park, Jieun Jang, Hojoon Choi, Jinbo Kim, Donggyun Kim, Kyubin Shim, Teahoon Park,\* Goomin Kwon\* and Jeonghun Kim\*

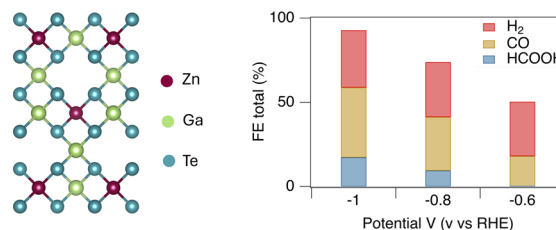


26364

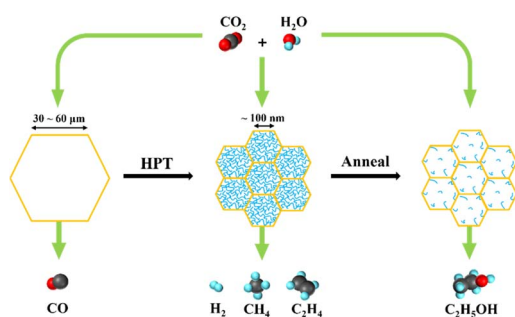
### ZnGa<sub>2</sub>Te<sub>4</sub> thin-film absorbers for photoelectrochemical CO<sub>2</sub> reduction

Shaham Quadir,\* Yungchieh Lai, Melissa K. Gish, John S. Mangum, Wayne Zhao, Ruo Xi Yang, Mona Abdelgaid, Christopher P. Muzzillo, Kristin A. Persson, Joel A. Haber, Sage R. Bauers and Andriy Zakutayev\*

### ZnGa<sub>2</sub>Te<sub>4</sub> Thin Film as a Photocathode



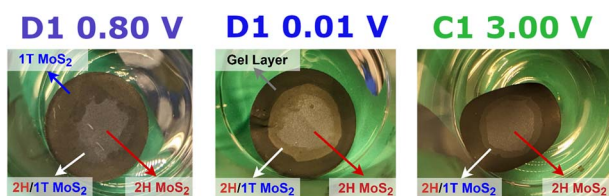
26377



### Effect of crystal defects on the selectivity of a bulk Cu–Zn alloy for electrocatalytic CO<sub>2</sub> reduction

Shengnan Hao, Peng Zhang, Yuying Meng, Wenbiao Zhang, Qingsheng Gao,\* Kaveh Edalati\* and Huai-Jun Lin\*

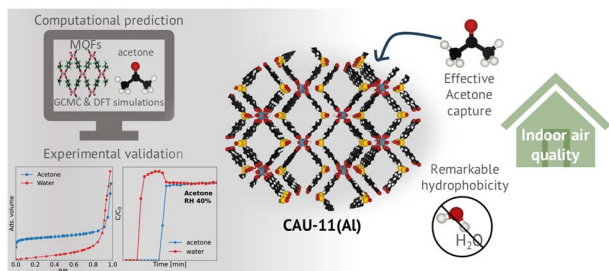
26389



### Visible lithiation gradients of bulk MoS<sub>2</sub> in lithium-ion coin cells

Alexandar D. Marinov, Ami R. Shah, Christopher A. Howard and Patrick L. Cullen\*

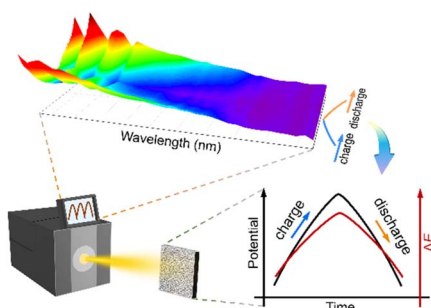
26401



### High-performance hydrophobic MOFs for selective acetone capture under humid conditions

Sabrina Grigoletto, Kavosh Karami, Iago Maye, Ajay Padunnappattu, Siddharth Ravichandran, Mohammad Wahiduzzaman, Louis Vanduyfhuys, Veronique Van Speybroeck, Matthias Thommes, Joeri F. M. Denayer, Norbert Stock\* and Guillaume Maurin\*

26413



### Replacing electrochemical measurement by colorimetric measurement to evaluate supercapacitor electrodes

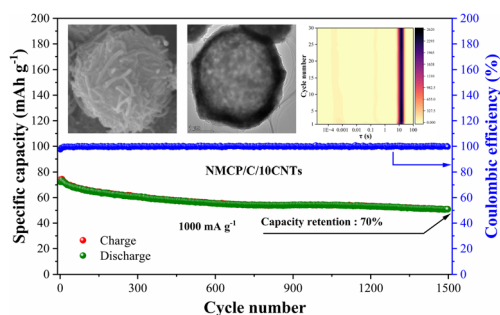
Yuanhui Su, Yu Huan,\* Wang Liu, Shuotong Wang, Xiaoying Guo and Tao Wei\*



26421

### Spray-drying synthesis of high-performance $\text{Na}_4\text{MnCr}(\text{PO}_4)_3$ for sodium-ion batteries via a CNT-induced conductive network and optimized interface kinetics

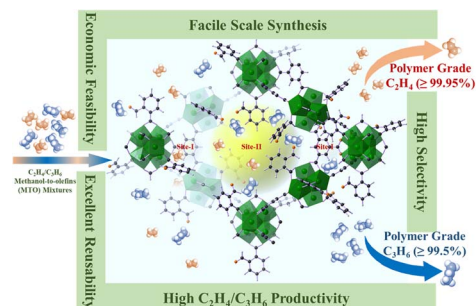
Suo Chen, Zidong Zhang, Jie Hou, Xin He, Qingyuan Wang, Zhanpeng Zhou, Wei Wang,\* Min Zhou, Kangli Wang and Kai Jiang\*



26431

### Site-engineered Zr-based metal–organic frameworks for ultrahigh-performance one-step separation of methanol-to-olefins products

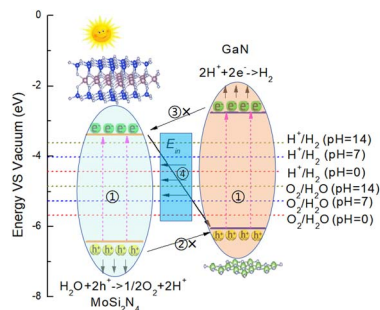
Jianfei Xiao, Jifei Ma, Zhenliang Zhu, Yaoqi Huang\* and Shaojun Yuan\*



26441

### Strain-tunable electronic and optical properties of a Z-scheme $\text{MoSi}_2\text{N}_4/\text{GaN}$ vdW heterojunction

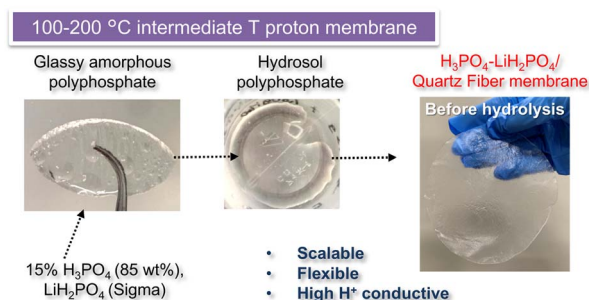
Shiquan Feng,\* Yifan Ma, Yang Yang, Shizhuo Wang, Xuechao Feng and Luogang Xie



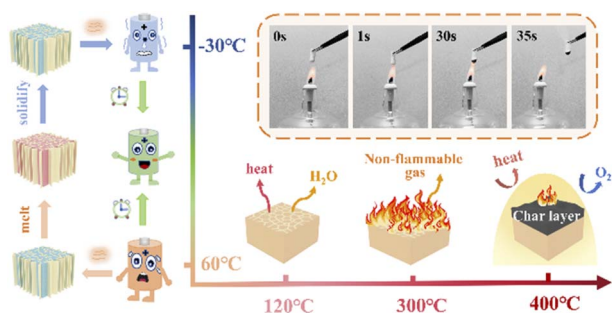
26448

### Highly conductive $\text{LiH}_2\text{PO}_4$ -based solid electrolyte at intermediate temperatures through a polymerization-hydrolysis treatment

Ke Xu, Keisuke Obata, Takaaki Suzuki, Kazuya Yamaguchi, Masao Katayama and Kazuhiro Takanabe\*



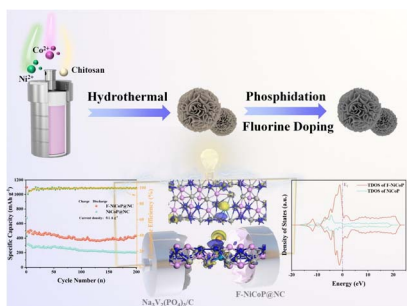
26458



### Orderly hybrid aerogel-based hydrate salt for wide-temperature range thermal regulation and flame retardancy in Li-ion batteries

Beibei Lei, Xiaoting Shen, Wei Chen, Ziyang Hong and Miao Wang\*

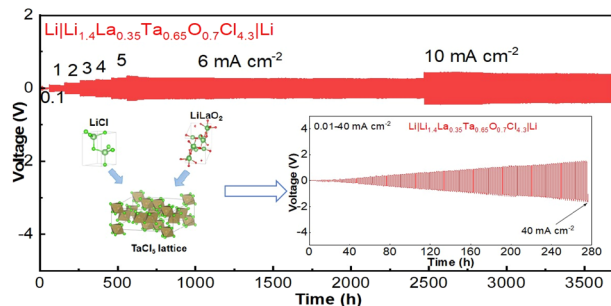
26467



### Fluorine-doping-induced phosphorus vacancy engineering in NiCoP@NC for enhanced sodium storage performance

Xinyue Liu, Shuling Liu,\* Qiangqiang Shi, Zijing Wu, Lulu Chen, Mingyue Zhang and Jianbo Tong\*

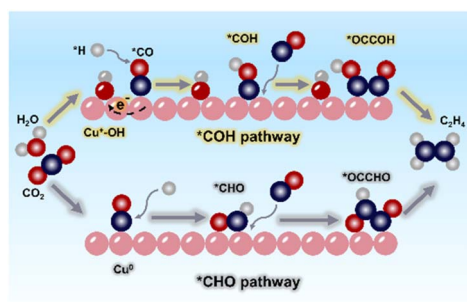
26478



### Amorphous oxyhalide solid electrolytes with improved ionic conductivity and reductive stability for all-solid-state batteries

Shufeng Song,\* Fengkun Wei, Wei Xue, Yanming Cui, Zhixu Long, Hongyang Shan and Ning Hu\*

26487



### Switching the formation of intermediates through inherent Cu<sup>+</sup>–OH structures over Cu-based catalysts for enhanced electrochemical CO<sub>2</sub> reduction to ethylene

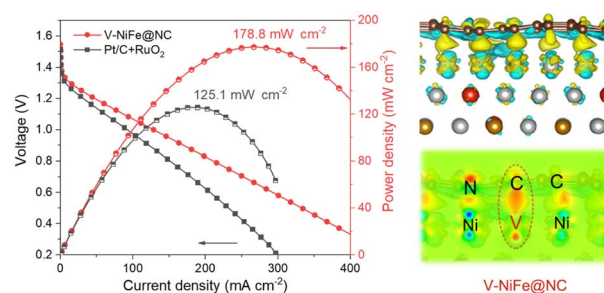
Zhijian Chen, Zhenghui Ma, Wenlin Yang, Guoli Fan,\* Baoming Ren and Feng Li\*



26499

## Optimizing the electronic structure of carbon-based NiFe nanoparticles *via* a vanadium mediated strategy for efficient oxygen reduction catalysts in Zn–air batteries

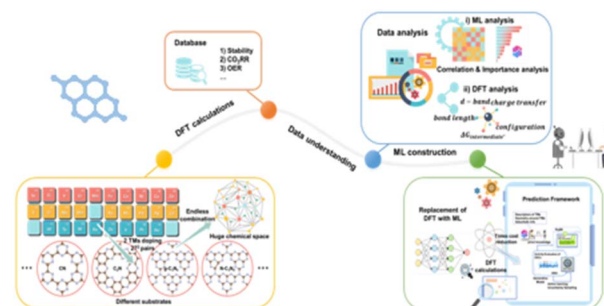
Ke Yang,\* Kun Zhu, Yawen Bo, Qihan Gong, Kebin Chi, Ziqin Yao, Sisi Cheng, Annayev Remezhan, Yan Li and Yu Yan\*



26509

## Data-guided design of double-atom catalysts for enhanced electrocatalytic performance

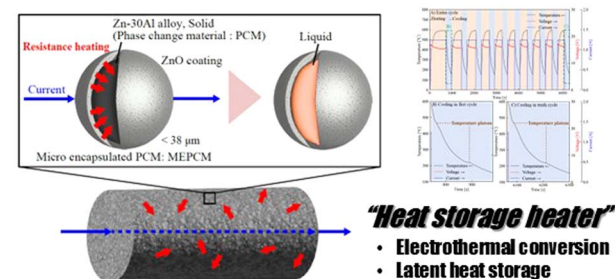
Chenyang Wei, Wenbo Mu,\* Hongyuan Zhang, Zhenghui Liu\* and Tiancheng Mu\*



26521

## Development of a heat storage heater for hybrid electrothermal conversion and latent heat storage

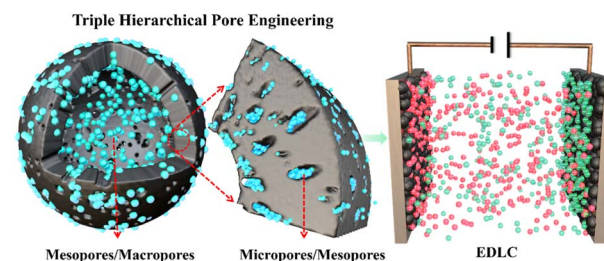
Takahiro Kawaguchi, Yusuke Sato, Joshua Chidiebere Mba, Yuto Shimizu, Kaixin Dong, Melbert Jeem and Takahiro Nomura\*



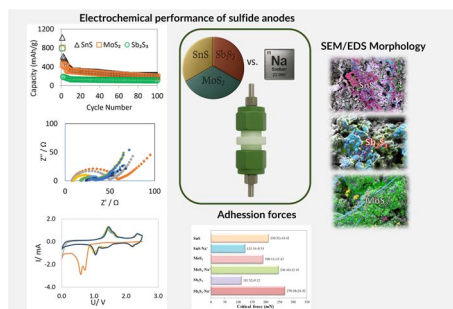
26534

## Rational engineering of triple-hierarchical pores in carbon nanospheres for superior organic supercapacitive storage

Zhenhu Li,\* Yongsu Li, Yaoning Tian, Jun Xiao, Feiyang Pan and Shuangyi Liu



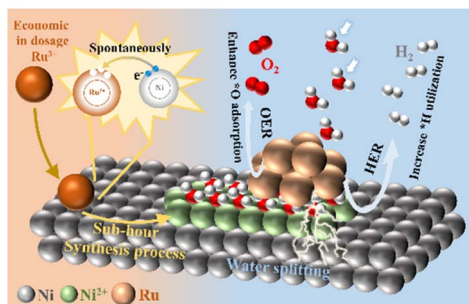
26544



### Electrochemical performance of MoS<sub>2</sub>, Sb<sub>2</sub>S<sub>3</sub>, and SnS anodes in sodium-ion batteries using a conductive polypyrrole-carbon black composite and an LBG sustainable binder

Ewelina Rudnicka,\* Aleksandra Mirowska, Manuela Skowron and Beata Kurc

26555

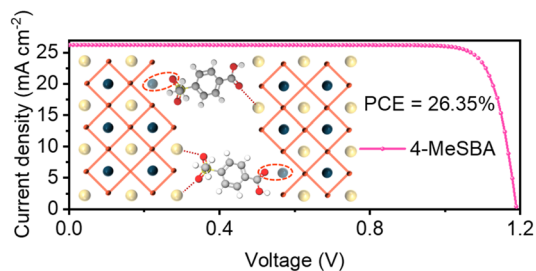


### Ultra-economical fabrication of a Ru cluster-loaded Ni(OH)<sub>2</sub> self-supported electrode *via* sub-hour corrosion for effective bifunctional water splitting

Junlei Qi, Rongrong Xu, Taili Yang, Mengting Yang, Jiping Chen, Jinchun Tu, Bingrong Wang, Chaoqun Qu, Zixuan Wang, Jian Cao and Yaotian Yan\*

26564

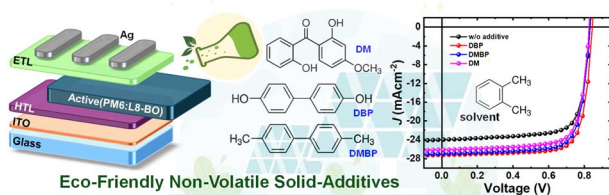
### Table of Contents Entry



### Molecular locking of defects *via* H-bonding/coordination dual-interaction enables efficient perovskite solar cells

Yansen Guo, Hailong Huang, Yiqing Zhang, Zewu Feng, Yanbo Wang, Jianjun Xu, Huanyu Zhang, Yi Ji, Le Li, Chenghao Ge, Xueqi Wu, Yitong Liu, Xin Li, Yige Peng, Chaopeng Huang, Yurou Zhang, Jingsong Sun, Siyu Chen, Weichang Zhou, Dongsheng Tang, Jefferson Zhe Liu, Klaus Weber, Youyong Li, Bin Ding, Hualin Zhan,\* Xiaohong Zhang and Jun Peng\*

26573



### Eco-friendly non-volatile solid additives for high-efficiency sustainable organic photovoltaic cells

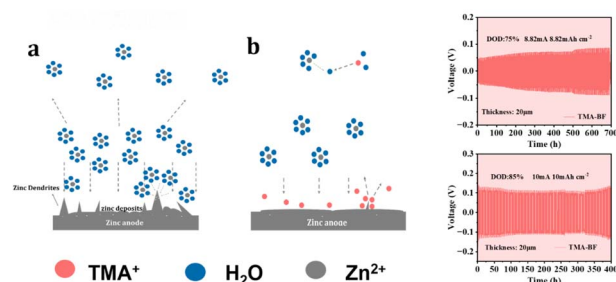
Do Hui Kim, Heunjeong Lee, Dongchan Lee, Jiwoo Yeop, Jin Young Kim and Shinuk Cho\*



26581

### Constructing highly reversible zinc batteries under high depth of discharge & current density conditions via quaternary ammonium cations modulating electric field force and competitive solvation

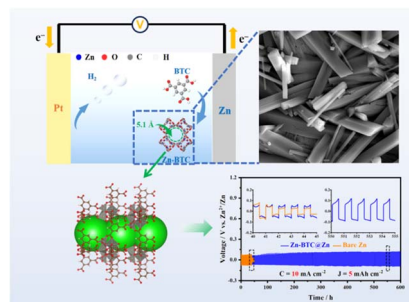
Ruizhe Zhang, Yongbo Fan,\* Jiayi Li, Zhiyong Liao, Zhuo Zhang, Peizhi Dong, Zexue Lin, Ning Yang and Huiqing Fan\*



26593

### A nanoconfinement-driven interface boosts zinc deposition kinetics toward dendrite-free zinc anodes

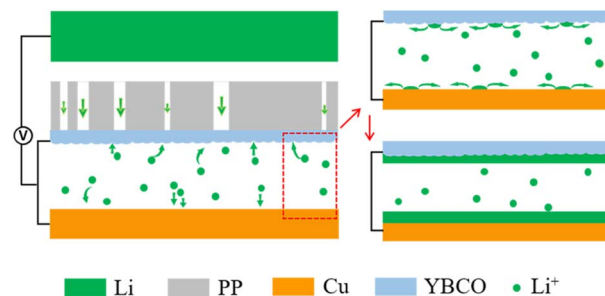
Qing Wen, Tian Chen, Chao Sun, Yujing Chen, Ruihan Ji, Rude Cui, Hezhang Chen, Linbo Tang, Jiafeng Zhang, Xiahui Zhang\* and Junchao Zheng\*



26601

### Lithophilic conductive oxide-introduced dual-substrate deposition for high current density lithium metal batteries

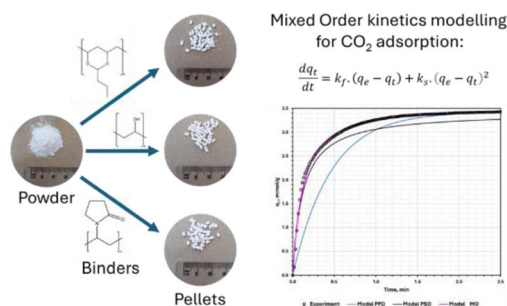
Juntao Si, Yida Wang, Jingchao Xiao, Yunyong Hu, Bicao Pan and Chunhua Chen\*



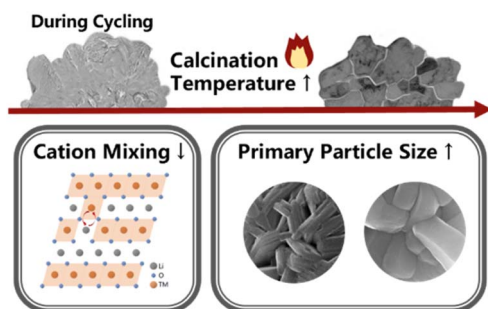
26610

### Kinetics of CO<sub>2</sub> adsorption on UTSA-16(Zn) metal-organic framework: thermal, compositional, and geometrical effects

Sanad Altarawneh and John Luke Woodliffe\*



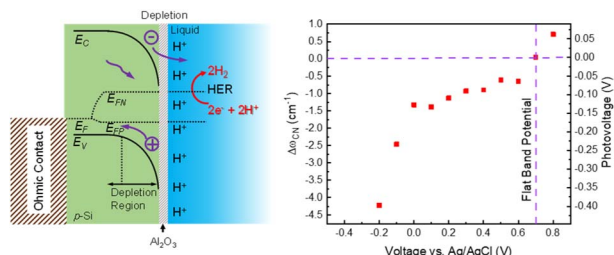
26627



### Origin of electrochemical cycling stability induced by calcination temperature for cobalt-free nickel-rich cathodes

Chenxi Song, Yaoyu Ren,<sup>\*</sup> Lin Gu, Qingyun Zhang, Yang Lu and Yang Shen<sup>\*</sup>

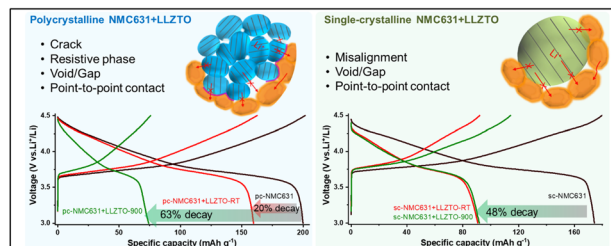
26637



### Monitoring photovoltages produced at semiconductor/liquid interfaces using *in situ* surface-enhanced Raman scattering (SERS) spectroscopy

Ruoxi Li, Yu Yun Wang, Sizhe Weng, Rifat Shahriar and Stephen B. Cronin<sup>\*</sup>

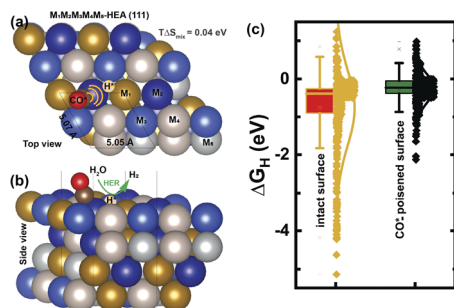
26647



### Thermal stability and electrochemical behavior of commercial polycrystalline and single-crystalline cathodes integrated with cubic $\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.6}\text{O}_{12}$ for all-solid-state lithium batteries

Ziting Ma, Grant LaBriola, Karlo Adrian Salazar, Chunting Chris Mi and Lingping Kong<sup>\*</sup>

26660



### Breaking the poisoning paradigm: a high-throughput DFT screening of high-entropy alloys with a focus on phonon-induced uncertainty

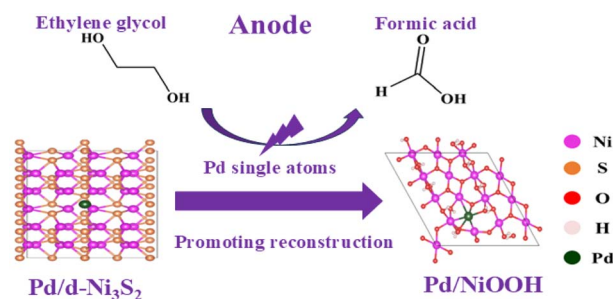
Mohsen Tamtaji, William A. Goddard III<sup>\*</sup> and GuanHua Chen<sup>\*</sup>



26669

### Anchoring Pd single atoms through S vacancies of defective nickel–sulfur for efficient electrocatalytic polyethylene terephthalate oxidation coupled with hydrogen evolution

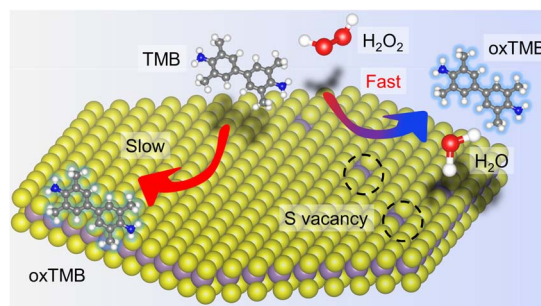
Mingming Zhan, Lipeng Guo, Xin Liang, Zhefei Zhao,\* Xingyu Luo, Ruopeng Yu, Qilong Wu, Linlin Zhang, Runtao Jin, Yihan Zhu, Yi Jia\* and Huajun Zheng\*



26681

### Synergistic construction of defect-rich nanozymes via montmorillonite support loading and iron doping for enhanced peroxidase-like activity

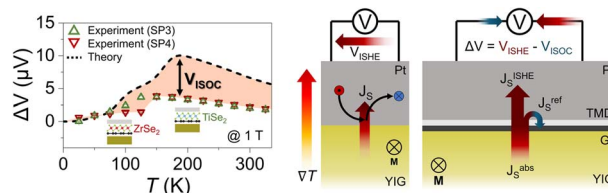
Wenjie Qu, Xiaorong Yang, Feng Feng, Yihe Zhang\* and Wangshu Tong\*



26690

### Negative spin-to-charge current induced by interfacial spin–orbit coupling in Pt/monolayer 1T-TiSe<sub>2</sub>/graphene/yttrium iron garnet quadruple heterostructures

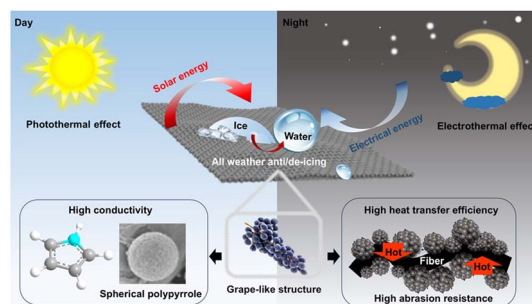
Jae Won Choi, Yun-Ho Kim, Jung-Min Cho, Katsuaki Sugawara, Jungtae Nam, Min-Sung Kang, Gangmin Park, Gil-Sung Kim, No-Won Park, Takashi Kikkawa, Won-Yong Lee, Young-Gui Yoon, Keun Soo Kim, Eiji Saitoh, Takafumi Sato\* and Sang-Kwon Lee\*



26700

### A robust grape-like superhydrophobic surface for efficient oil–water separation and anti/de-icing

Xiaoyan Xu, Chutong Xiao, Wenquan Liu, Wei Li,\* Lingling Feng, Xixuan Fang and Hui Qiao\*

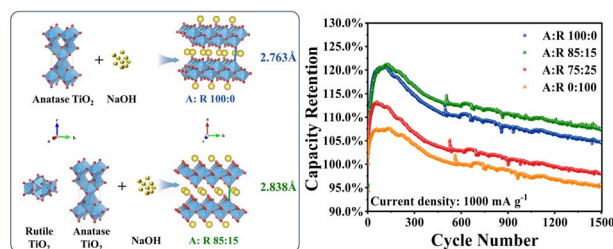




26756

### The balance of structural compatibility and distortion in titanium sources for the preparation of a high performance $\text{Na}_2\text{Ti}_6\text{O}_{13}$ anode

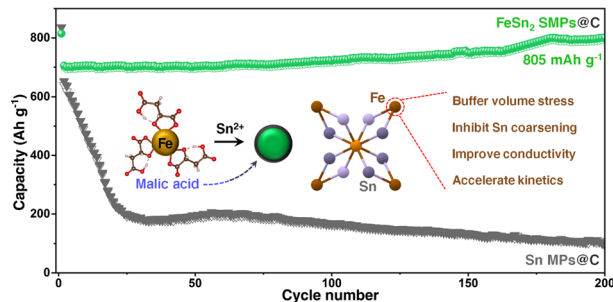
Qian Li, Changyan Hu, Yihua Liu, Ruoyang Wang, Feng Chen, Tingru Chen, Zhenguo Wu\* and Xiaodong Guo



26764

### A robust malic acid-assisted displacement reaction to form carbon-coated submicron $\text{FeSn}_2$ with superior lithium storage reversibility enabled by the solid solution effect

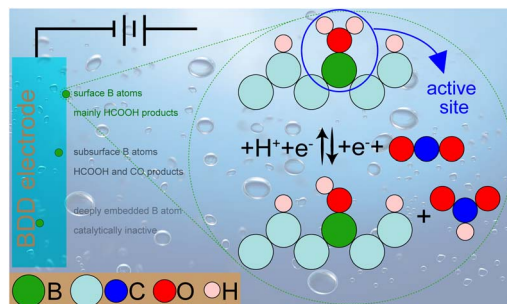
Guanghui Li, Chunhua Jiang, Shuaiwei Sun, Dongli Pei, Guangqiang Ma, Huile Jin, Shiqiang Zhao,\* Shun Wang\* and Xiaoxu Bo\*



26779

### Boron site-dependent electrocatalytic $\text{CO}_2$ reduction at the boron-doped diamond– $\text{H}_2\text{O}$ interface

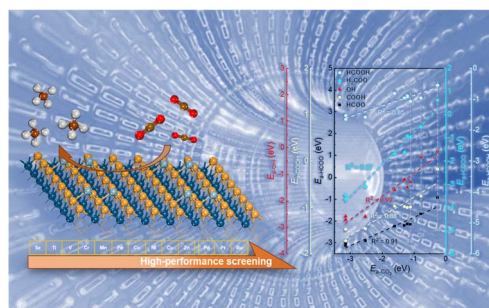
Kai Zhu, Shaohua Lu and Xiaojun Hu\*



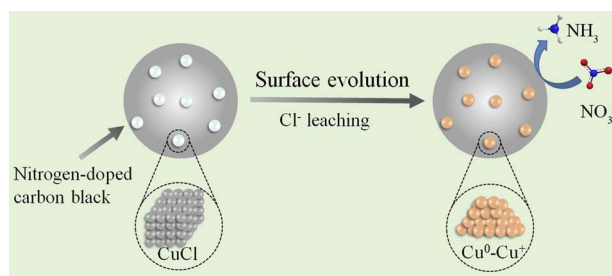
26788

### Rational design of $\text{MoS}_2$ -based dual-atom catalysts for $\text{CO}_2$ -to-methane conversion: thermodynamic and electronic insights into activity and selectivity

Yuxiang Jin, Zhengtong Ji, Xue Yao, Erhong Song\* and Yongfu Zhu\*



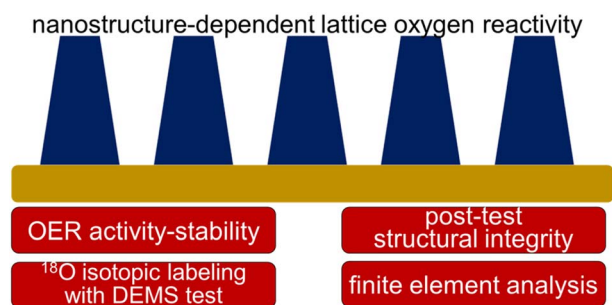
26797



### Anion leaching induced amorphous Cu/CuO<sub>x</sub> on N-doped carbon for efficient electrochemical nitrate reduction to ammonia

Maolin Zhang, Karthik Peramaiah, Moyu Yi and Hao Huang\*

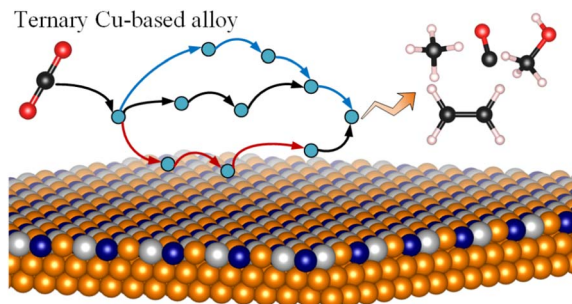
26804



### Nanostructure-dependent lattice oxygen reactivity and degradation of CoNi oxyhydroxide OER electrocatalysts: a mechanistic study

Liuyuan Ran, Kai Zhao, Xiaoyi Jiang and Ning Yan\*

26812



### A convenient method of ternary alloys design for CO<sub>2</sub>-to-C<sub>2</sub>H<sub>4</sub> electroreduction

Yiyang Xiao, Yingju Yang,\* Wei Liu and Jing Liu

