

# Journal of Materials Chemistry A

Materials for energy and sustainability

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## IN THIS ISSUE

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### Cover

See Zhipeng Gao *et al.*, pp. 31127–31134. Image reproduced by permission of Zhipeng Gao from *J. Mater. Chem. A*, 2024, 12, 31127.

## EDITORIAL

30941

### Introduction to Frontiers in Electrocatalysis for Clean Energy

Ahsanulhaq Qurashi,\* Anders Hagfeldt, Kelsey A. Stoerzinger and Huang Yizhong

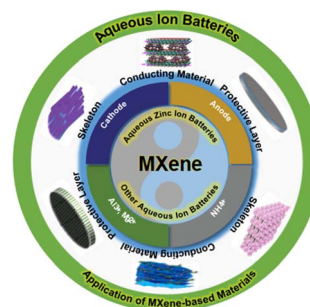


## REVIEWS

30944

### MXene-based materials: potential high-performance electrodes for aqueous ion batteries

Xiru Chen, Zhen Wang,\* Sensen Xue, Weixin Guan, Ligu Gao, Tingli Ma, Xuefeng Ren,\* Anmin Liu\* and Xifei Li\*



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# EES Batteries

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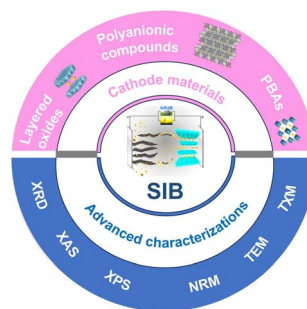
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30971

### Advances in sodium-ion battery cathode materials: exploring chemistry, reaction mechanisms, and prospects for next-generation energy storage systems

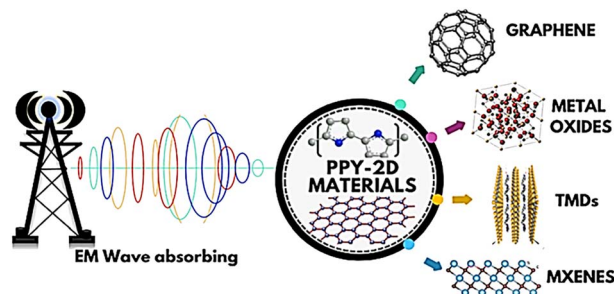
Han Zhang, Liguang Wang\* and Pengjian Zuo\*



31004

### Microwave absorbing properties of polypyrrole-based 2D nanocomposites

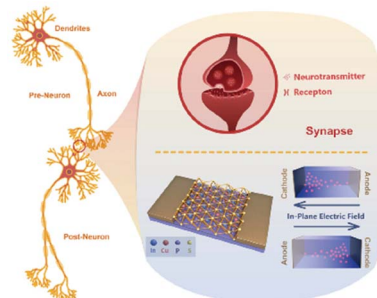
Raeesah Islam, Yuvika Sood, Harish Mudita, Anil Ohlan and Anil Kumar\*



31028

### Emerging van der Waals material $\text{CuInP}_2\text{S}_6$ : physical properties, theories and applications

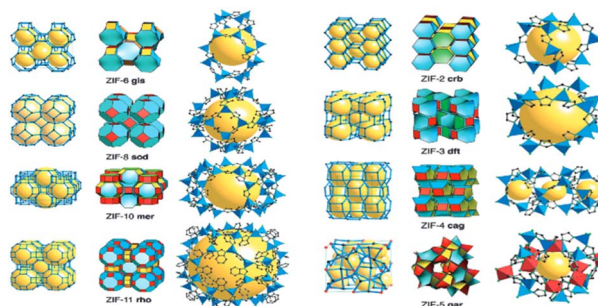
Tian-Xiao Xu, Xiao-Bing Guo,\* Dan Zhang, Qi-Jun Sun, Yan-Ping Jiang, Qiu-Xiang Liu and Xin-Gui Tang\*



31059

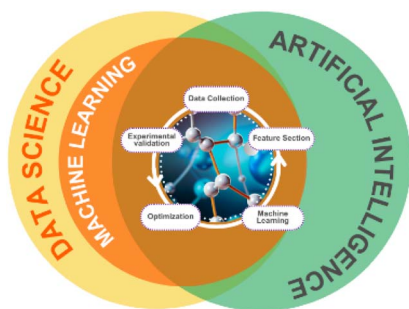
### Application and prospects of metal-organic frameworks in photocatalytic self-cleaning membranes for wastewater treatment

Haolan Xiao, Zezhen Zhang, Shuman Feng, Xinyi Wang and Lili Wu\*



## REVIEWS

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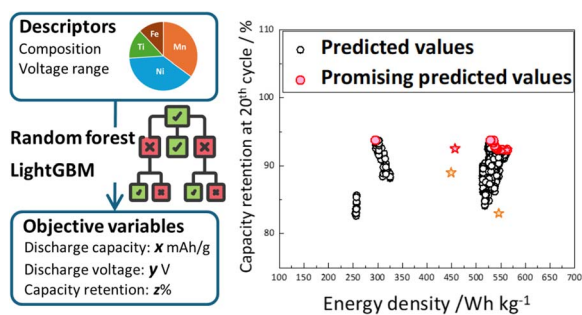


### AI and ML for selecting viable electrocatalysts: progress and perspectives

Anastasiia P. Dmitrieva, Anna S. Fomkina, Chantal T. Tracey, Elizaveta A. Romanenko, Ali Ayati, Pavel V. Krivoschapkin and Elena F. Krivoschapkina\*

## COMMUNICATIONS

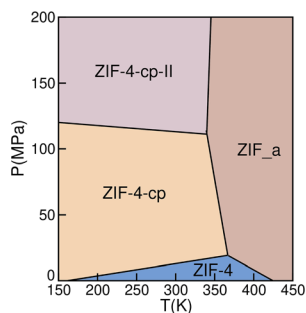
31103



### Na[Mn<sub>0.36</sub>Ni<sub>0.44</sub>Ti<sub>0.15</sub>Fe<sub>0.05</sub>]O<sub>2</sub> predicted via machine learning for high energy Na-ion batteries

Saaya Sekine, Tomooki Hosaka, Hayato Maejima, Ryoichi Tatara, Masanobu Nakayama and Shinichi Komaba\*

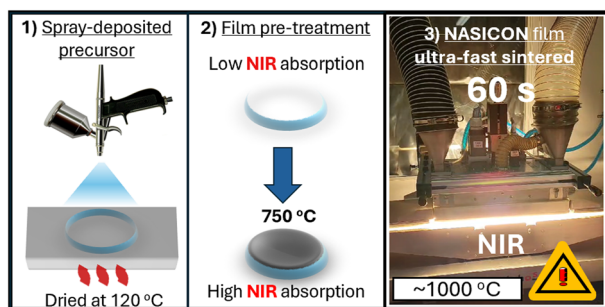
31108



### Phase diagram of ZIF-4 from computer simulations

Emilio Méndez and Rocio Semino\*

31116



### A new approach for obtaining ceramic NASICON (Na<sub>3</sub>Zr<sub>2</sub>Si<sub>2</sub>PO<sub>12</sub>) films sintered *in situ* by a sol-gel method, using spray deposition and near-infra red sintering

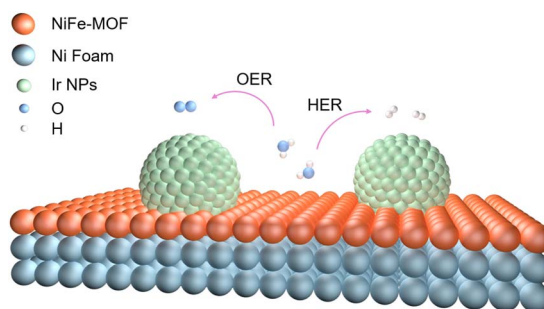
Rafael Marti Valls, Rebecca Griffin, Anne Sawhney, Celina Domingos-Dlofo, Tom Dunlop, Sam Reis, Peter J. Holliman and Jenny Baker\*



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### Ir nanoparticles decorated NiFe metal–organic framework as a highly efficient and stable heterostructure electrocatalyst for overall seawater splitting

Hefeng Wang, Zixiao Li, Zhengwei Cai, Chaoxin Yang, Shengjun Sun, Xiaoyan Wang, Min Zhang, Meng Yue, Dongdong Zheng, Asmaa Farouk, Mohamed S. Hamdy, Xuping Sun\* and Bo Tang\*

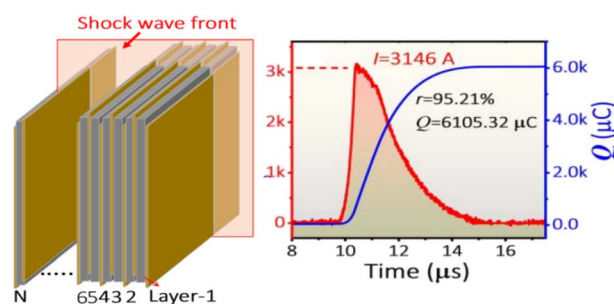


PAPERS

31127

### Ultrahigh output energy density of explosive-energy-conversion devices assembled from multilayer ferroelectric films

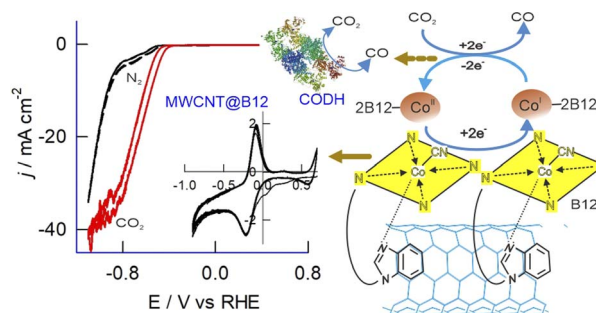
Zhengwei Xiong, Zhangyang Zhou, Yi Liu, Zhengqian Fu, Fangfang Xu, Leiming Fang, Xiaoru Liu, Jun Li, Ke Jin and Zhipeng Gao\*



31135

### Enzyme-mimicking redox-active vitamin B12 functionalized MWCNT catalyst for nearly 100% faradaic efficiency in electrochemical CO<sub>2</sub> reduction

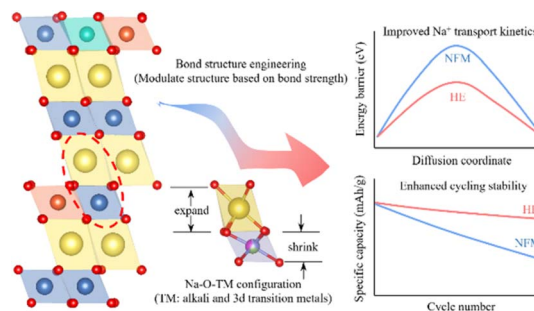
Yashly Yesudas K., Mani Balamurugan, Ki Tae Nam, Buvaneswari Gopal\* and Annamalai Senthil Kumar\*



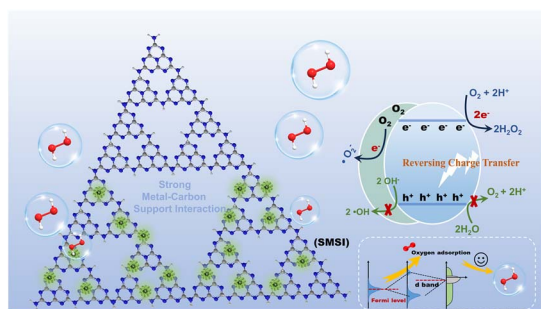
31145

### Redox and structural stability for sodium-ion batteries through bond structure engineering

Xingyu Li, Yi Li, Qinwen Cui, Minghui Zhong, Xiaolin Zhao\* and Jianjun Liu\*



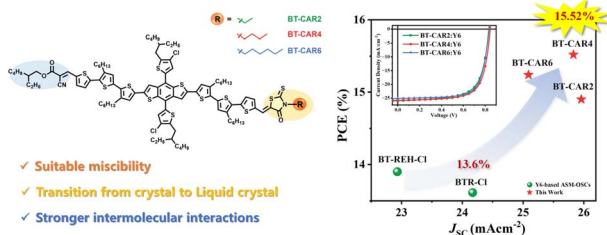
31153



### Strong metal–support interaction (SMSI) modulates d-orbital centers to promote oxygen reduction reaction

Zhangmeng Liu, Guiting Lin, Yayao Li, Runchao Zhou and Yunzhi Fu\*

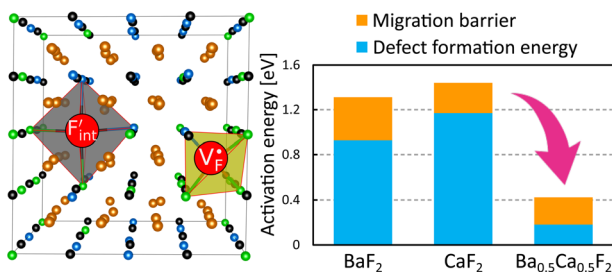
31163



### Asymmetric liquid crystalline donors with two different end groups enable efficient all-small-molecule organic solar cells

Chenhe Wang, Tianyi Chen, Shuixing Li,\* Yecheng Shen, Jinyang Yu, Adiljan Wupur, Yongmin Luo, Mengting Wang, Xiukun Ye, Jiaying Wu, Minmin Shi\* and Hongzheng Chen\*

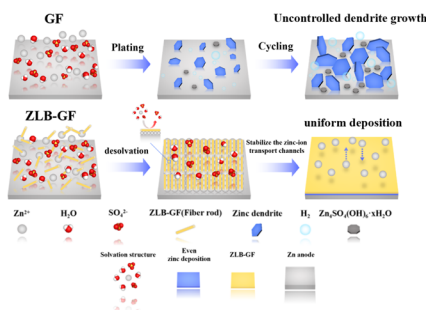
31173



### Point-defect chemistry for ionic conduction in solid electrolytes with isovalent cation mixing

Takafumi Ogawa,\* Kazuyuki Sato, Kazuhiro Mori, Shunsuke Kobayashi, Hiroki Moriwake, Yuichi Ikuhara and Akihide Kuwabara

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### Zein improved GF separator for dendrite-free aqueous zinc-ion batteries

Bozhong Cao, Qian Qu, Bingchun Jiang, Tianyu Zou, Shubing Zhen, Peiwen Wang, Kairui Li, Jincheng Zhang, Hui Guo and Tong Zhang\*

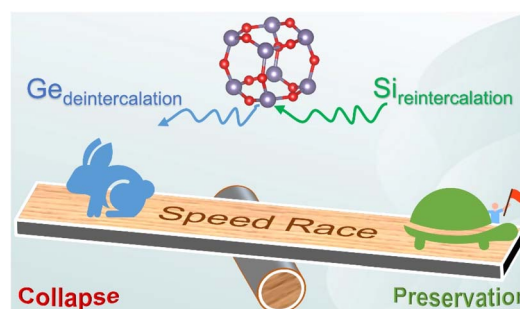




31195

## Balancing Ge de-intercalation and Si re-insertion rates stabilizes hydrolytically labile germanosilicate zeolites

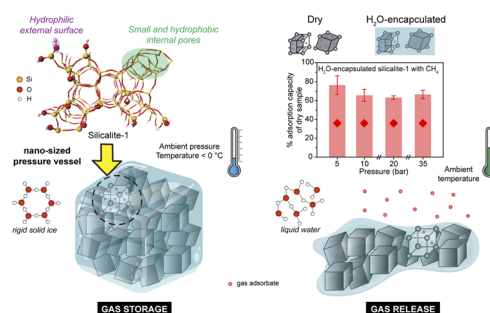
Jin Zhang, Qiudi Yue, Emad Shamma, Sarra Abdi, Oleg Petrov, Jiří Čejka, Svetlana Mintova, Maksym Opanasenko\* and Mariya Shamzhy



31204

## Gas storage within nanoporous material encapsulated by ice

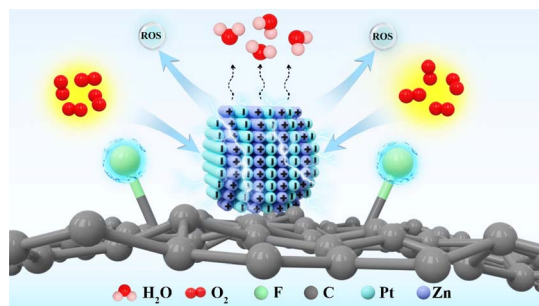
Jia Ming Goh, Zhi Yu, Ali Zavabeti, Shuangmin Shi, Yalou Guo, Jianan He, Jianing Yang, Lei Dong, Paul A. Webley, Amanda Vera Ellis and Gang Kevin Li\*



31214

## A potential well effect for efficient oxygen reduction and corrosion resistance under the operating temperature conditions of PEMFCs

Chang Li, Yiyang Mao, Ji Qiu, Xixi Wang, Jie Miao, Yulin Min,\* Wei Zhou\* and Zongping Shao\*

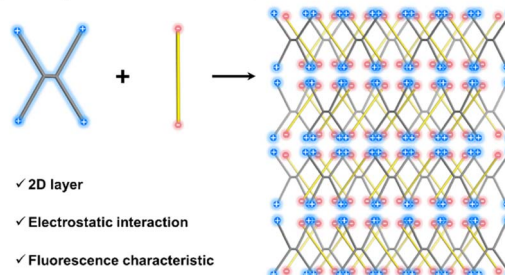


31223

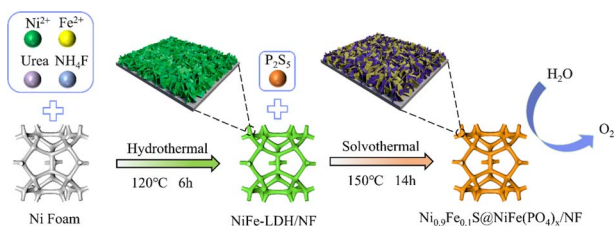
## A 2D layered fluorescent crystalline porous organic salt

Danling Sun, Guolong Xing,\* Jie Lyu, Yuxia Han, Pu Sun, Yu Zhao, Kanwal Iqbal, Huating Kong, Yuanbin Zhang, Daoling Peng,\* Bo Song, Weidong Zhu and Teng Ben\*

### A 2D Layered Fluorescent CPOS



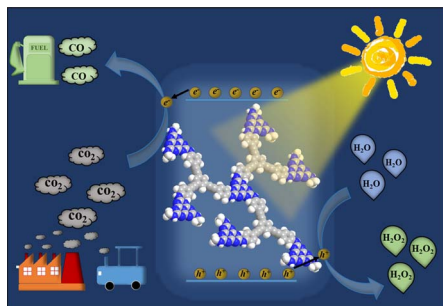
31233



### Iron-doped nickel sulfide@phosphate heterostructure nanosheets constructed from solvothermal $P_2S_5$ and layered double hydroxides for electrocatalytic oxygen evolution

Zeyi Wang, Shuling Liu,\* Chenglong Wang, Dan Ren, Yanling Hu, Yujie Ma and Chao Wang\*

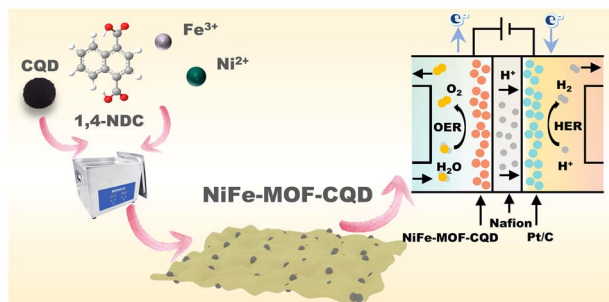
31244



### Molecular engineering of donor–acceptor heptazine-based porous organic polymers for selective photoreduction of $CO_2$ to $CO$ under non-sacrificial conditions in water

Amit Kumar, Pravesh Kumar, Durgesh Pandey, Neha Saini, Kirti Dhingra, Dibyajyoti Ghosh and Kamalakannan Kailasam\*

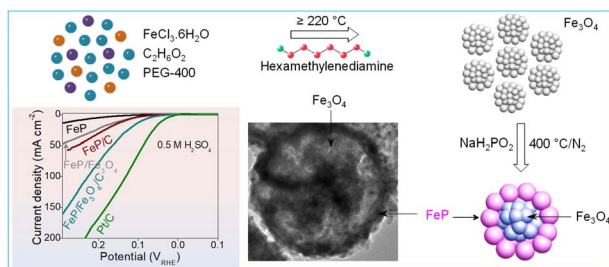
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### Carbon quantum dot-mediated binary metal–organic framework nanosheets for efficient oxygen evolution at ampere-level current densities in proton exchange membrane electrolyzers

Qianjia Ni, Shiyuan Zhang, Kang Wang, Huazhang Guo, Jiye Zhang, Minghong Wu and Liang Wang\*

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### Ultrathin carbon layer-coated mesoporous core–shell-type FeP/Fe $_2$ O $_3$ /C for the hydrogen evolution reaction

Alaaldin Adam, María Isabel Díez-García, Joan Ramon Morante, Muhammad Ali, Zijin Chen, Ziqi Tian and Mohammad Qamar\*

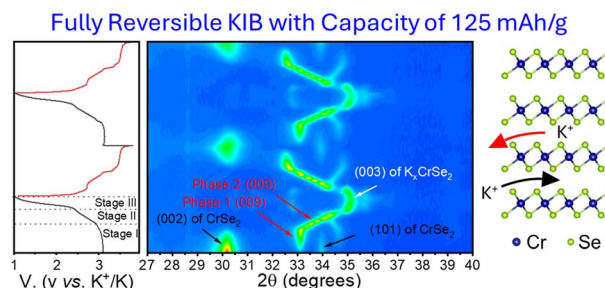




31276

## Reversible K-ion intercalation in CrSe<sub>2</sub> cathodes for potassium-ion batteries: combined *operando* PXRD and DFT studies

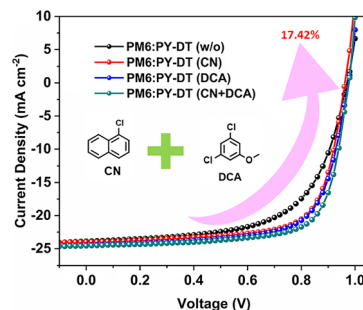
Weihao Li, Johannes Döhn, Jinyu Chen, Manuel Dillenz, Mohsen Sotoudeh, David M. Pickup, Shunrui Luo, Ryan Parmenter, Jordi Arbiol, Maria Alfredsson, Alan V. Chadwick, Axel Groß, Maider Zarrabeitia\* and Alexey Y. Ganin\*



31284

## High performance all-polymer solar cells enabled with solvent and solid dual additives

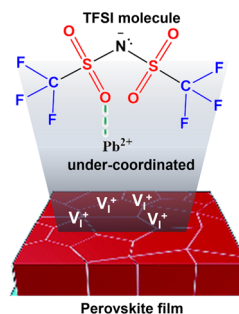
Misbah Sehar Abbasi, Congqi Li, Jinhua Gao, Siying Wang, Sixuan Wang, Qijie Lin, Gening Xie, Saqib Nawaz Khan, Jianqi Zhang, Xin Zhang, Yunhao Cai\* and Hui Huang\*



31291

## Influence of TFSI post-treatment on surface doping and passivation of lead halide perovskites

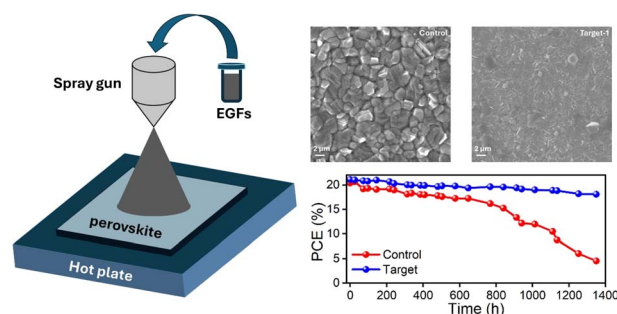
Konstantina Gkini, Spyros Orfanoudakis, Filippos Harlaftis, Panagiotis Dallas, Christos Kouzios, Polychronis Tsipas, Athanassios G. Kontos, Maria Konstantakou and Thomas Stergiopoulos\*



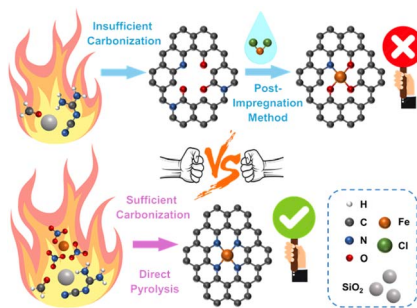
31301

## Stable perovskite solar cells with exfoliated graphite as an ion diffusion-blocking layer

Abdullah S. Alharbi, Miqad S. Albishi, Temur Maksudov, Tariq F. Alhuwaymel, Chrysa Aivalioti, Kadi S. AlShebl, Naif R. Alshamrani, Furkan H. Isikgor, Mubarak Aldosari, Majed M. Aljomah, Konstantinos Petridis, Thomas D. Anthopoulos, George Kakavelakis\* and Essa A. Alharbi\*



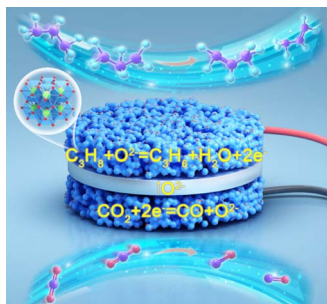
31312



### Comparing direct pyrolysis and post-impregnation in the synthesis of atomic Fe active sites for solvent-free aerobic coupling of benzylamine

Guilong Lu, Zewen Shen, Philipp Schwiderowski, Jannik Böttger, Tim Herrendorf, Wolfgang Kleist, Xiaoyu Li, Guixia Zhao, Baoxiang Peng, Xiubing Huang\* and Martin Muhler\*

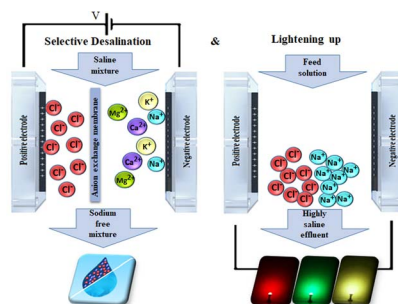
31323



### Electrochemical oxidative dehydrogenation of propane to propylene in an oxygen-ion conducting solid oxide electrolyzer

Cong Luo, Jiaming Ma, Lingting Ye\* and Kui Xie\*

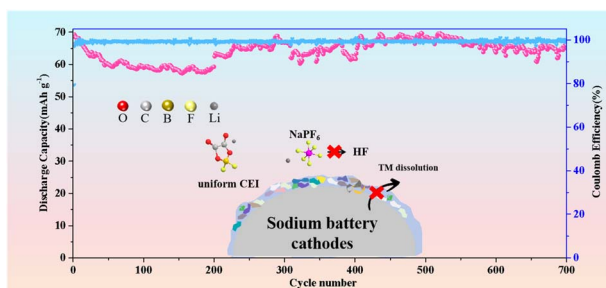
31329



### Towards an advanced electrochemical horizon: ion selectivity and energy harnessing through hybrid capacitive deionization with carbon-coated NaTi<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> and N-rich carbon nests

Hanieh Sharifpour, Farzaneh Hekmat,\* Saeed Shahrokhian\* and Likun Pan

31347



### Construction of a stable interface at the Na<sub>0.67</sub>Ni<sub>0.33</sub>Mn<sub>0.67</sub>O<sub>2</sub> cathode using LiDFOB electrolyte additives for high-performance sodium-ion batteries

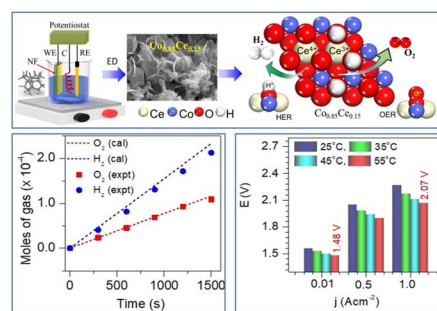
Siyao Li, Hui Xu,\* Yuanqiang Zhu, Ziwei Yang, Yuanhai Bao and Yong Chen\*



31362

### Cobalt oxide/cerium oxide heterogeneous interfaces as advanced durable and bifunctional electrocatalysts for robust industrially relevant overall water splitting

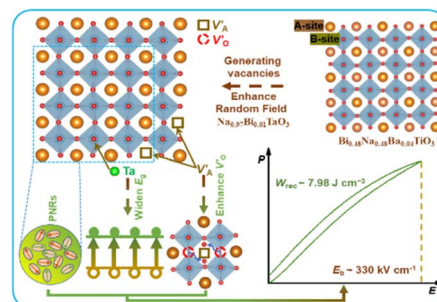
Akbar I. Inamdar,\* Amol S. Salunke, Jun Ho Seok, Harish S. Chavan, Nabeen K. Shrestha, Sang Uck Lee,\* Sangeun Cho\* and Hyunsik Im



31375

### Excellent low-field energy storage properties and high density achieved in $\text{Bi}_{0.48}\text{Na}_{0.48}\text{Ba}_{0.04}\text{TiO}_3$ -based oxide ceramics via interposing $(\text{Na}_{0.97}\text{Bi}_{0.01})^+/\text{Ta}^{5+}$ at A/B sites

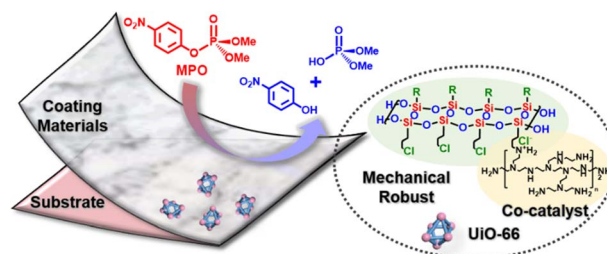
Jiwei Du, Tianhui Shi, Qin Feng,\* Ronghao Jia, Jianan Hu, Changlai Yuan,\* Xinpeng Wang, Xiyong Chen, Nengneng Luo and Jiwei Zhai\*



31386

### Robust surface coating materials for chemical warfare agent simulant detoxification using ladder-like poly(silsesquioxane) and metal-organic framework composites

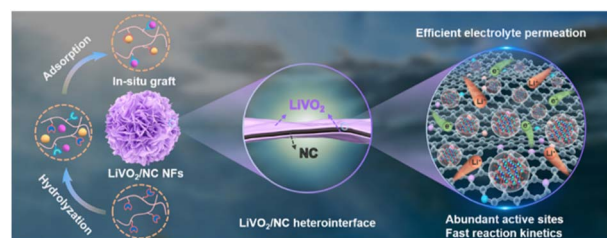
Seungjae Lee, Seungjae Hur, Keunhong Jeong, Hoesun Hwang, Jungkyu Choi, Nithima Khaorapapong, Kyung-Youl Baek, Jin Young Seo,\* Yusuke Yamauchi and Jongbeom Na\*



31396

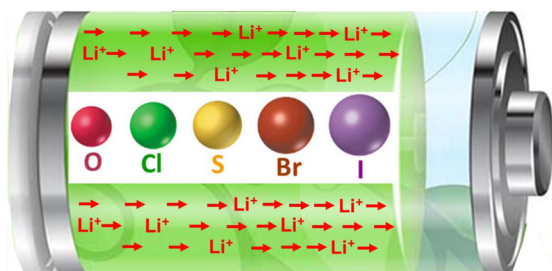
### Flower-like carbon-confined disordered rock-salt $\text{LiVO}_2$ anode with a sandwich structure for fast charging and stable lithium storage

Sicong Shen, Bing Sun,\* Xiaomeng Bai, Song Yang, Dongmei Zhang, Cunyuan Pei, Pengju Li and Shibing Ni\*





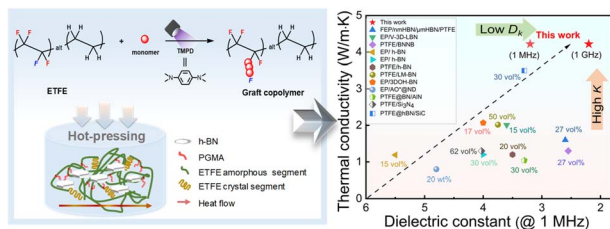
31405

"Increasing Li<sup>+</sup> ions conductivity with halogen elements"

**Incorporation of halogens (Cl, Br, and I) in an Li–P–S–O system for exploring new sulfide solid electrolytes with high conductivity and superior electrochemical performance in solid-state batteries**

Hari Raj, Audric Neveu, Christian Jordy, Vincent Pelé and Valerie Pralong\*

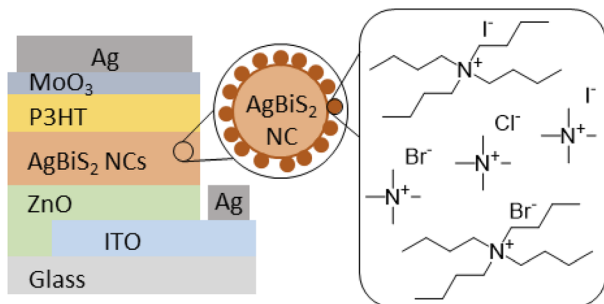
31424



**Optimizing thermal and dielectric properties of ethylene-tetrafluoroethylene (ETFE)/h-BN composites *via* interface engineering: activation of C–F bonds on ETFE for surface grafting**

Miao Wang, Yijin He, Xiaoyu Yang, Xuhui Hou, Wenxuan Li, Shaobo Tan\* and Zhicheng Zhang\*

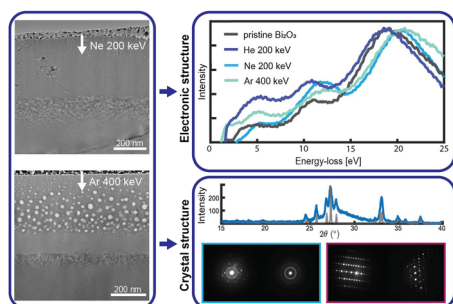
31432



**Effect of different halide-based ligands on the passivation and charge carrier dynamics in AgBiS<sub>2</sub> nanocrystal solar cells**

Fiona Treber, Elke De Grande, Ute B. Cappel and Erik M. J. Johansson\*

31445



**Insights into defect kinetics, mass transport, and electronic structure from spectrum effects in ion-irradiated Bi<sub>2</sub>O<sub>3</sub>**

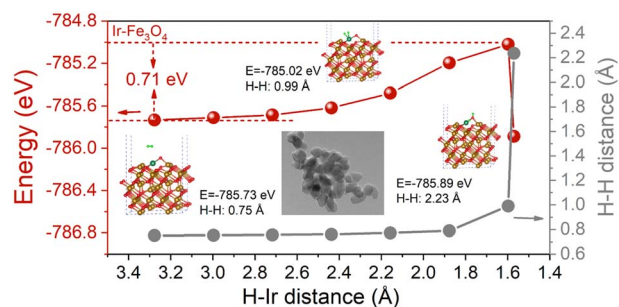
Ellis Rae Kennedy,\* James A. Valdez, Yongqiang Wang, Stephanie M. Ribet, Kurt E. Sickafus, Cortney R. Kreller, Blas Pedro Uberuaga and Benjamin K. Derby



31459

## Understanding the catalysis of noble metals in reduction of iron oxide by hydrogen: insights from DFT calculations

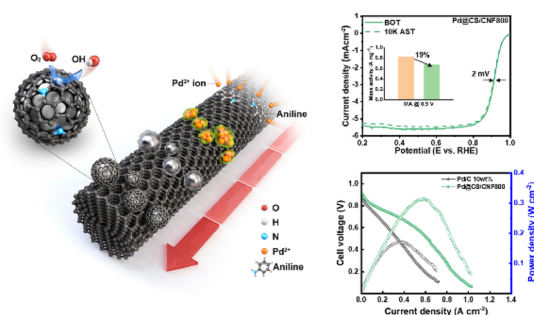
Qiming Tang, Xueling Lei,\* Yongliang Zhang, Jiabin Lu and Kevin Huang\*



31467

## A high-durability palladium catalyst for the oxygen reduction reaction in an alkaline environment

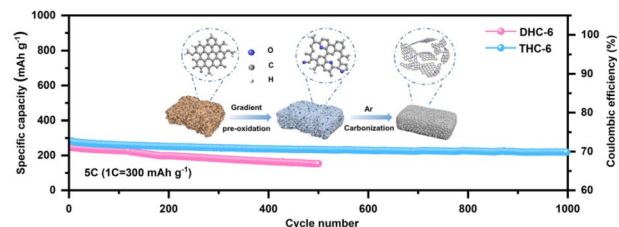
Hyo Eun Bae, Ji Eun Park, T. B. Ngoc Huynh, Jihyeok Song, Sung Ki Cho, Yung-Eun Sung,\* Yong-Hun Cho\* and Oh Joong Kwon\*



31480

## A molecular-scale regulation strategy for designing asphalt-based hard carbon for superior sodium storage

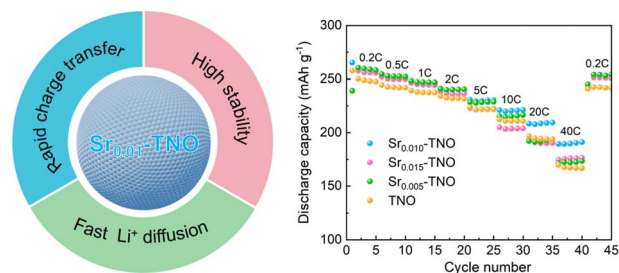
Ling Sheng, Peng Wei, He Ma, Shaoyang Wu, Kang Liang, Jianbin Li,\* Qi Wan\* and Yurong Ren\*



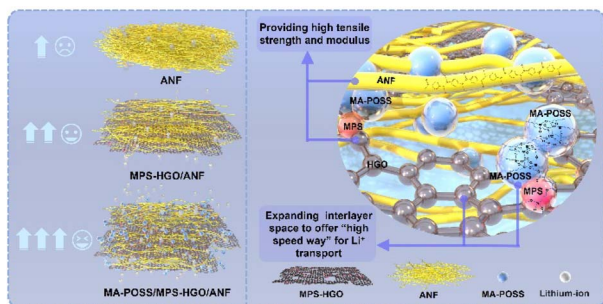
31492

## Sr-dopant microstructure engineering enables strong pseudocapacitive effects of TiNb<sub>2</sub>O<sub>7</sub> anode for fast-charging lithium-ion batteries

Wei Fang, Shenglu Geng, Anran Shi, Long Zang, Hailu Liu, Enjie Dong, Guolong Wu, Hongyu Zhao, Lingling Zhang,\* Geping Yin\* and Shuaifeng Lou\*



31500



### An ultrathin phase-inversion induced co-assembly separator for high-performance lithium-metal batteries

Yuying Wang, Fanjun Guo, Mengzhen Zhou, Qian Wu, Tao You, Zhengxiang Zhong, Jiankun Yang, Li Liu, Yudong Huang\* and Mingqiang Wang\*

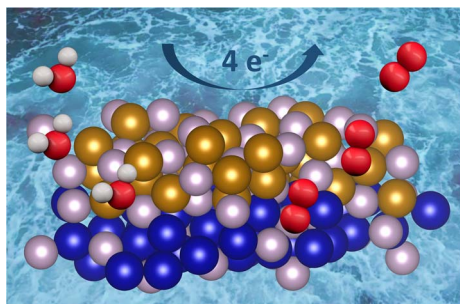
31508



### A reversed strategy for designing high-performance anode materials from a traditional $\text{Na}_x\text{V}_2\text{O}_5$ cathode

Jing Yao, Meichun He, Pengju Li,\* Chao Zhu, Dongmei Zhang, Cunyuan Pei, Bing Sun and Shibing Ni\*

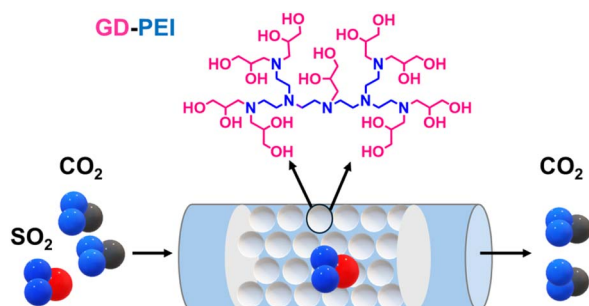
31518



### Electron redistribution induced by p-d orbital hybridization in $\text{Co}_2\text{P}/\text{FeP}$ nanosheets boosts water electrooxidation

Qiyang Sun, Yu Miao, Ruixue Zhang, Guang-Rui Xu,\* Chuanfang Zhang, Kang Liu, Zexing Wu and Lei Wang\*

31526



### Glycidol-modified PEI: a highly selective adsorbent for $\text{SO}_2$ in the presence of $\text{CO}_2$

Chanjot Kaur and Abdelhamid Sayari\*

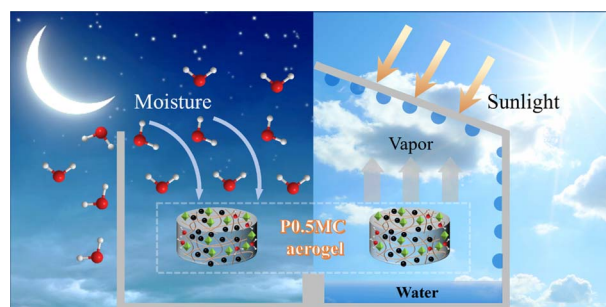




31533

### Engineering defective MOF-801 nanostructures on the surface of a calcium alginate aerogel for efficient and stable atmospheric water harvesting

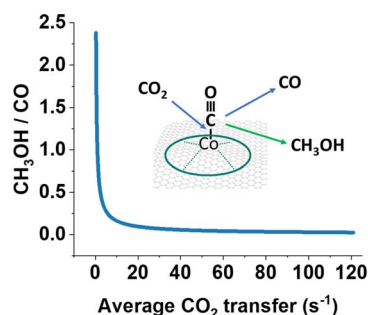
Cai-Hua Liu, Lei Xu,<sup>\*</sup> Zhen-Yu Wang, Sheng-Jie Han, Yi-Bin Li, Ming-Lai Fu<sup>\*</sup> and Baoling Yuan<sup>\*</sup>



31547

### Low CO<sub>2</sub> mass transfer promotes methanol and formaldehyde electrosynthesis on cobalt phthalocyanine

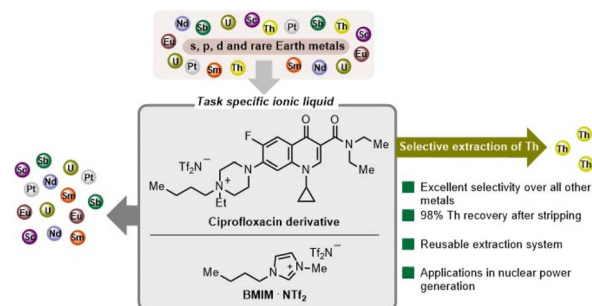
Jie Zhang, Thi Ha My Pham, Shibo Xi, Liping Zhong, David Liem, Futian You, Ben Rowley, Ramesha Ganganahalli, Federico Calle-Vallejo<sup>\*</sup> and Boon Siang Yeo<sup>\*</sup>



31557

### A ciprofloxacin derived task specific ionic liquid as a highly selective extractant of thorium versus uranium

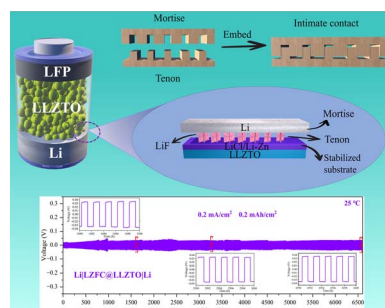
David Lledó, Guillermo Grindlay, H. Q. Nimal Gunaratne, Abel de Cózar, Ana Sirvent and José M. Sansano<sup>\*</sup>



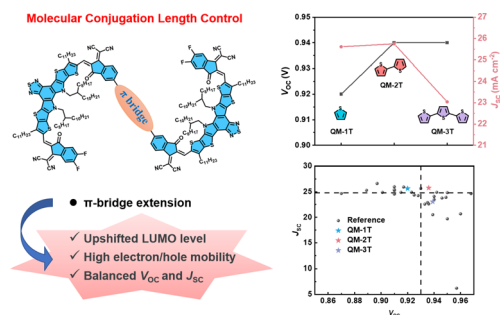
31570

### A mortise–tenon-like ionic/electronic conductive interface facilitates long-cycle solid-state lithium metal batteries

Guoxiang Zheng, Yifan Jin, Michal Sedlačik, Elif Vargun, Yifan Zhang, Ying He,<sup>\*</sup> Petr Saha and Qilin Cheng<sup>\*</sup>



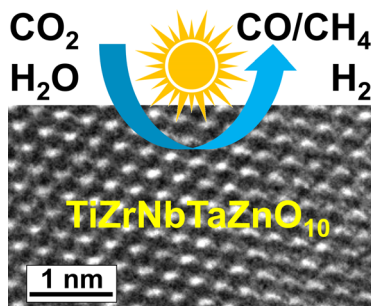
31581



### A- $\pi$ -A type quasi-macromolecular acceptors with molecular conjugation length control strategy for high-performance organic solar cells

Siqing He, Changhao Xiang, Wei Liu, Songting Liang, Rui Zhang, Weikun Chen, Bin Zhao, Jun Yuan\* and Yingping Zou

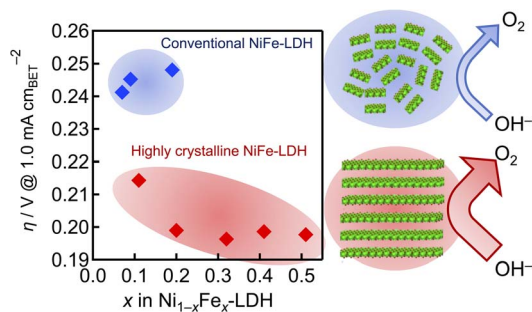
31589



### Hybrid $d^0$ and $d^{10}$ electronic configurations promote photocatalytic activity of high-entropy oxides for CO<sub>2</sub> conversion and water splitting

Jacqueline Hidalgo-Jiménez, Taner Akbay, Xavier Sauvage, Lambert van Eijck, Motonori Watanabe, Jacques Huot, Tatsumi Ishihara and Kaveh Edalati\*

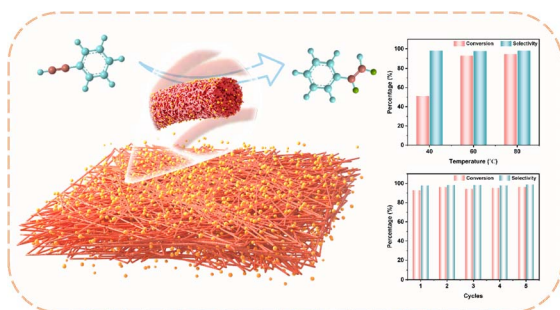
31603



### Superior oxygen evolution reaction activities of highly crystalline $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ ( $0.20 \leq x \leq 0.51$ ) synthesized using soft chemistry

Atsunori Ikezawa,\* Shinji Koito and Hajime Arai

31612



### Electron-deficient Pd nanoparticles on nitrogen-doped carbon nanofibers for high selectivity alkyne transfer semi-hydrogenation

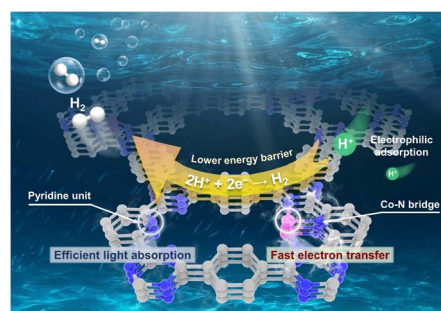
Huaike Li, Shuai Li, Guichu Yue, Songwei Gao, Xuefeng Zhang, Keping Zhu, Tingting Yang, Ziyue Zhang, Nü Wang, Jie Bai, Zhimin Cui\* and Yong Zhao\*



31619

### A pyridine-woven covalent organic framework facilitating the immobilization of Co single atoms towards efficient photocatalytic H<sub>2</sub> evolution

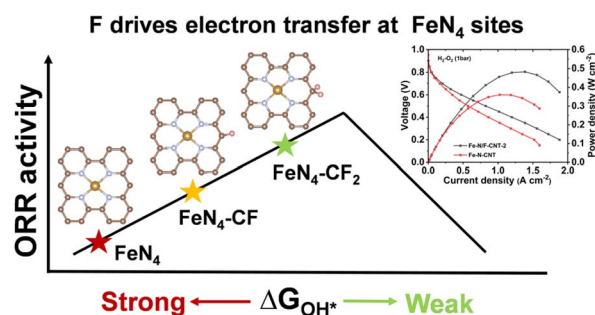
Yanchi Yao, Jingbo Lin, Shasha Liu, Yong Zheng, Lun Lu, Qile Fang, Shuang Song, Chao Zhu\* and Yi Shen\*



31630

### Boosting the ORR activity in PEM fuel cells: tailored electron-withdrawing properties of Fe-based catalysts via optimizing fluorine doping

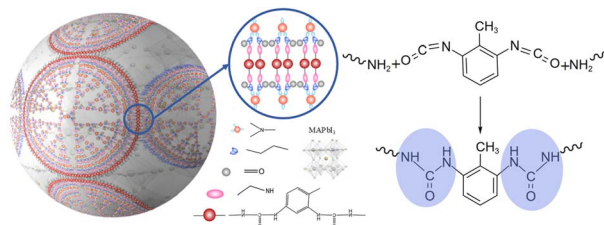
Nan Xue, Jian Yin, Xueyan Xue, Hui Zhu\* and Jiao Yin\*



31638

### Stable and flexible FP-RRAM with an *in situ* covalently constructed 3D dendritic framework

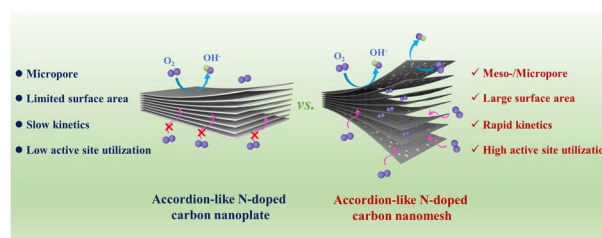
Mengru Liu, Xueqing Ma, Qianyu Zhao, Zhenya Li, Yingliang Liu,\* Shengang Xu and Shaokui Cao



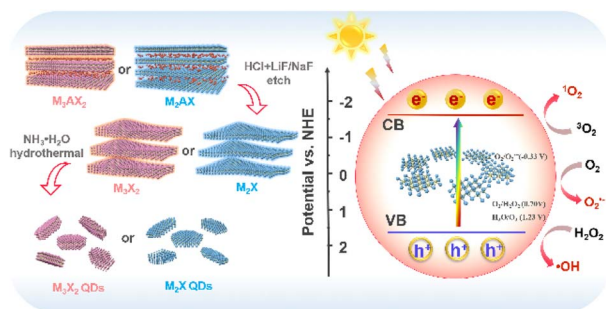
31647

### Multilayer meso–microporous carbon nanomesh: an effective oxygen reduction electrocatalyst

Fuping Zhang, Chenchen Ji,\* Chunmei Deng, Yinglin Zhang, Tingting Wei, Bo Xing, Liang Jiang, Yi Wang, Guo Yang and Yulin Shi\*







## Outstanding ROS generation ability and the mechanism of MXene quantum dots

Danyang Xiao, Chunxiao Wu, Bufeng Liang, Shangzuo Jiang, Jianxiong Ma\* and Yan Li\*

