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Journal of Materials Chemistry A

Materials for energy and sustainability

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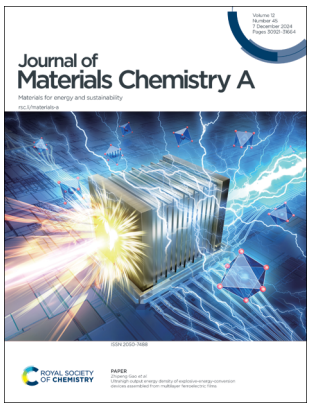
IN THIS ISSUE

ISSN 2050-7488 CODEN JMCAET 12(45) 30921–31664 (2024)



Cover
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EDITORIAL

30941

Introduction to Frontiers in Electrocatalysis for Clean Energy

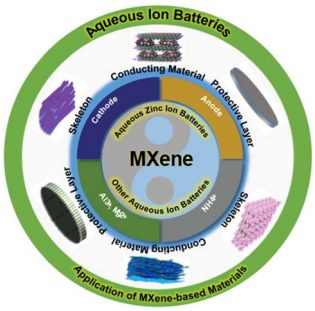
Ahsanulhaq Qurashi,* Anders Hagfeldt, Kelsey A. Stoerzinger and Huang Yizhong

REVIEWS

30944

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

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



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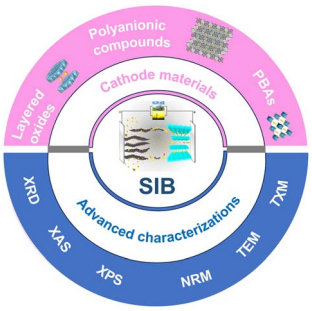
REVIEWS

30971

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

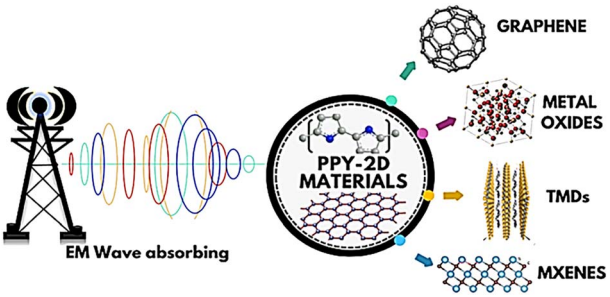
Han Zhang, Liguang Wang* and Pengjian Zuo*



31004

Microwave absorbing properties of polypyrrole-based 2D nanocomposites

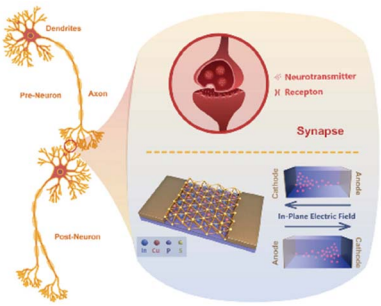
Raeesah Islam, Yuvika Sood, Harish Mudila, Anil Ohlan and Anil Kumar*



31028

Emerging van der Waals material $CuInP_2S_6$: physical properties, theories and applications

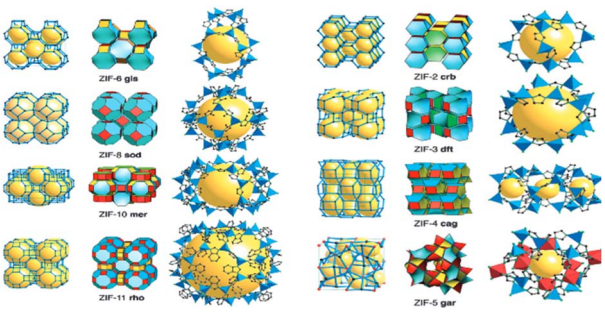
Tian-Xiao Xu, Xiao-Bing Guo,* Dan Zhang, Qi-Jun Sun, Yan-Ping Jiang, Qiu-Xiang Liu and Xin-Gui Tang*



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*



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REVIEWS

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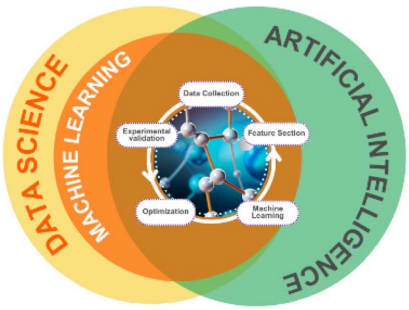
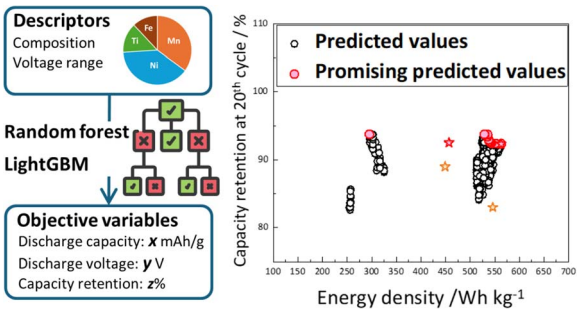


AI and ML for selecting viable electrocatalysts: progress and perspectives

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

COMMUNICATIONS

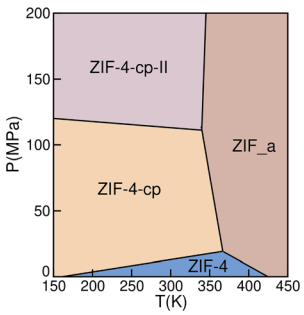
31103



$Na[Mn_{0.36}Ni_{0.44}Ti_{0.15}Fe_{0.05}]O_2$ predicted *via* machine learning for high energy Na-ion batteries

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

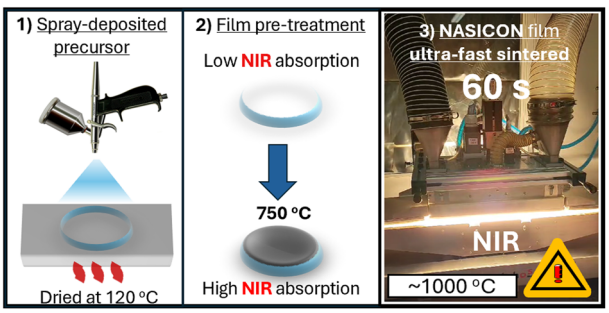
31108



Phase diagram of ZIF-4 from computer simulations

Emilio Méndez and Rocio Semino*

31116



A new approach for obtaining ceramic NASICON ($Na_3Zr_2Si_2PO_{12}$) 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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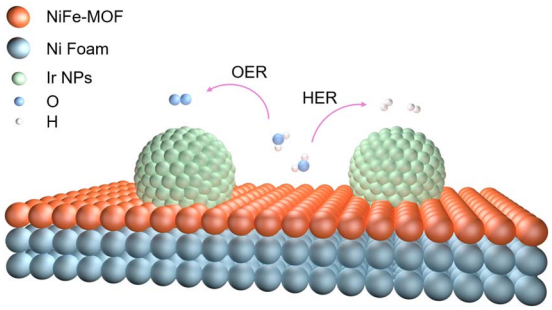
COMMUNICATIONS

31121

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*

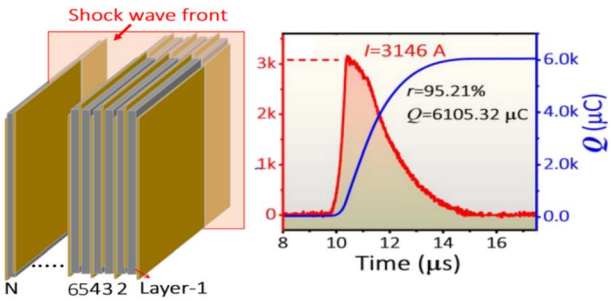


PAPERS

31127

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

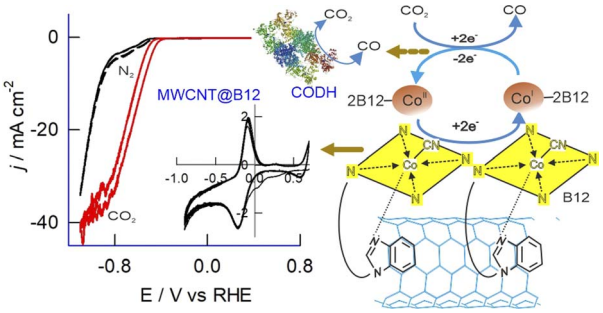
Zhengwei Xiong, Zhangyang Zhou, Yi Liu, Zhengqian Fu, Fangfang Xu, Leiming Fang, Xiaoru Liu, Jun Li, Ke Jin and Zhipeng Gao*



31135

Enzyme-mimicking redox-active vitamin B12 functionalized MWCNT catalyst for nearly 100% faradaic efficiency in electrochemical CO_2 reduction

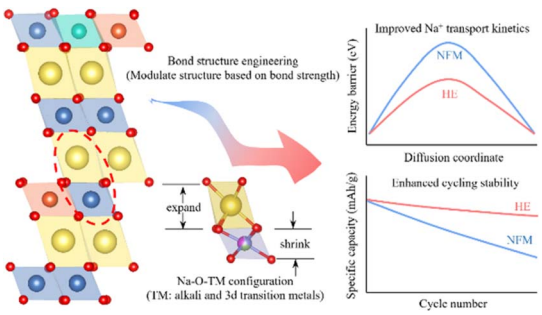
Yashly Yesudas K., Mani Balamurugan, Ki Tae Nam, Buvaneswari Gopal* and Annamalai Senthil Kumar*



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*



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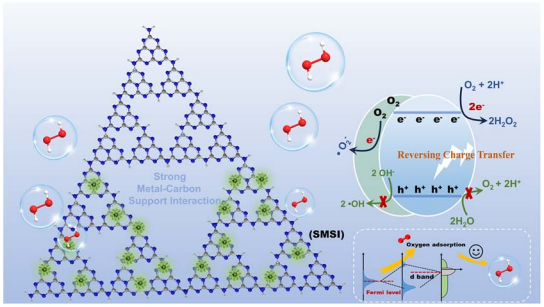
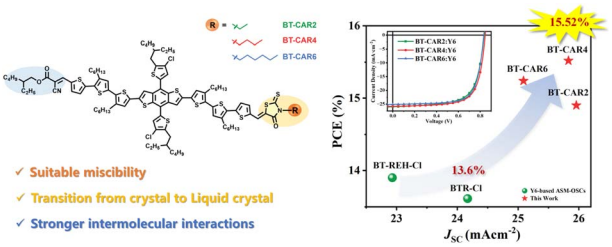


Strong metal–support interaction (SMSI) modulates d-orbital centers to promote oxygen reduction reaction

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

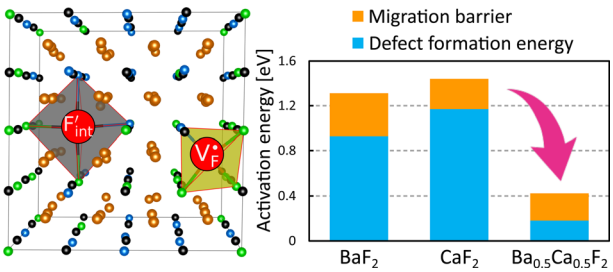
31163



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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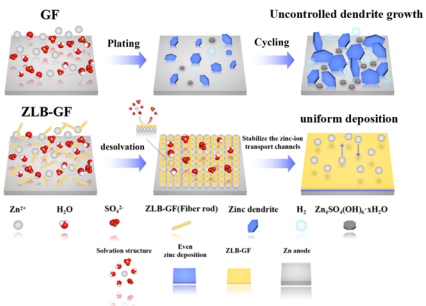

Zein improved GF separator for dendrite-free aqueous zinc-ion batteries

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

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PAPERS

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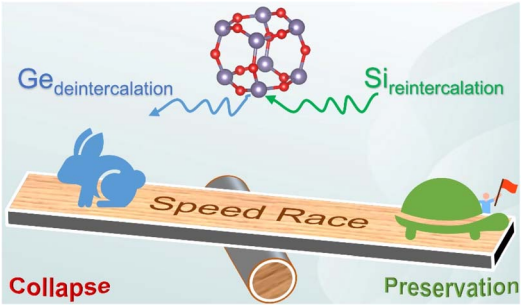
Balancing Ge de-intercalation and Si re-insertion rates stabilizes hydrolytically labile germanosilicate zeolites

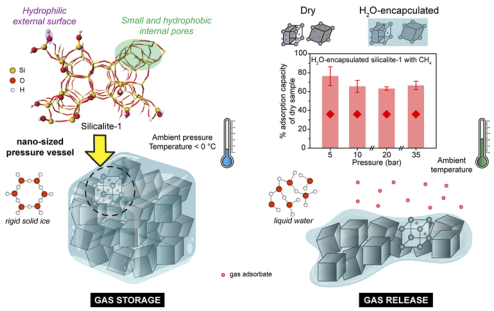
Jin Zhang, Qiudi Yue, Emad Shamma, Sarra Abdi, Oleg Petrov, Jiří Čejka, Svetlana Mintova, Maksym Opanasenko* and Mariya Shamzhy



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*



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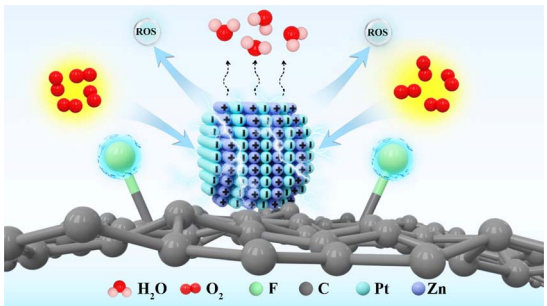
A potential well effect for efficient oxygen reduction and corrosion resistance under the operating temperature conditions of PEMFCs

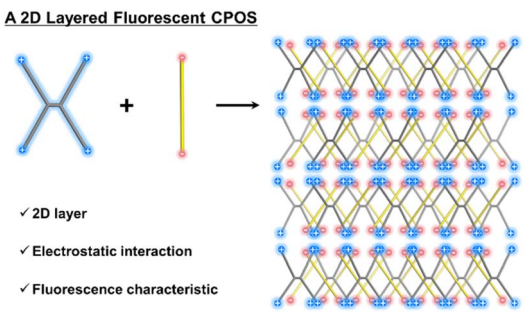
Chang Li, Yiyang Mao, Ji Qiu, Xixi Wang, Jie Miao, Yulin Min,* Wei Zhou* and Zongping Shao*



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*



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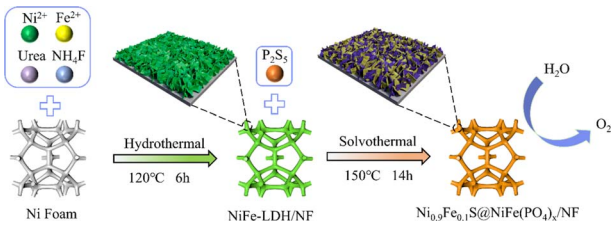
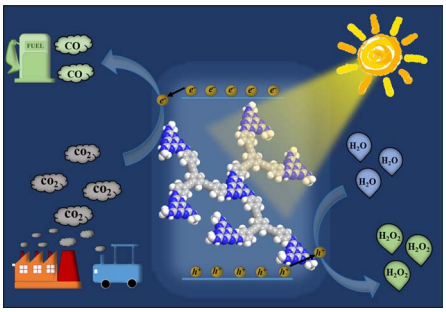


Iron-doped nickel sulfide@phosphate heterostructure nanosheets constructed from solvothermal P_2S_5 and layered double hydroxides for electrocatalytic oxygen evolution

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

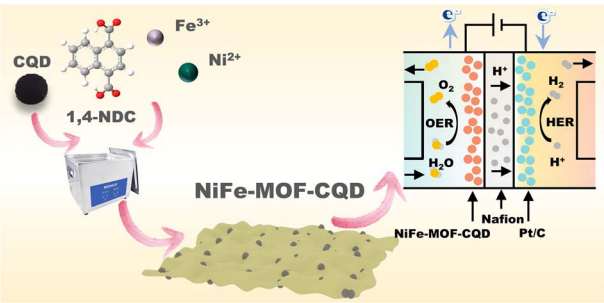
31244



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*

31253



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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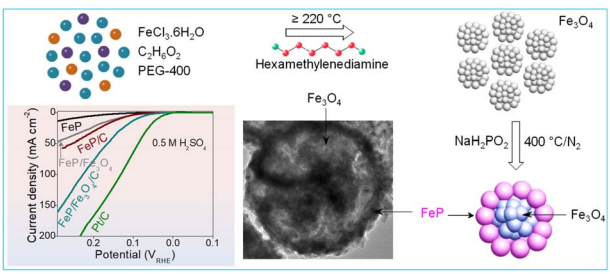

Ultrathin carbon layer-coated mesoporous core–shell-type $FeP/Fe_2O_3/C$ for the hydrogen evolution reaction

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

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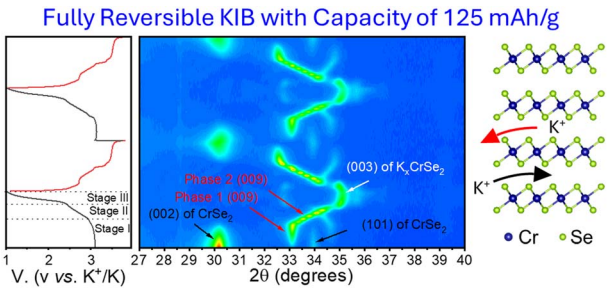
Reversible K-ion intercalation in $CrSe_2$ cathodes for potassium-ion batteries: combined *operando* PXRD and DFT studies

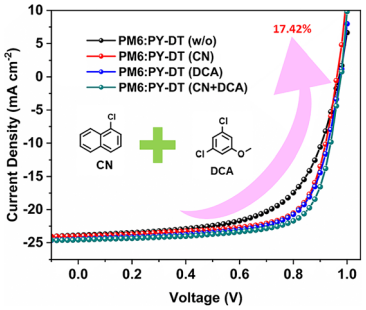
Weihao Li, Johannes Döhn, Jinyu Chen, Manuel Dillenz, Mohsen Sotoudeh, David M. Pickup, Shunrui Luo, Ryan Parmenter, Jordi Arbiol, Maria Alfredsson, Alan V. Chadwick, Axel Groß, Maider Zarrabeitia* and Alexey Y. Ganin*



31284

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

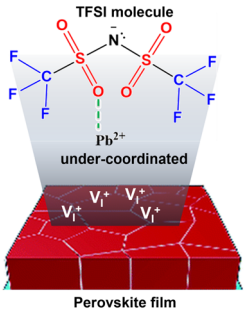
Misbah Sehar Abbasi, Congqi Li, Jinhua Gao, Siying Wang, Sixuan Wang, Qijie Lin, Gening Xie, Saqib Nawaz Khan, Jianqi Zhang, Xin Zhang, Yunhao Cai* and Hui Huang*



31291

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

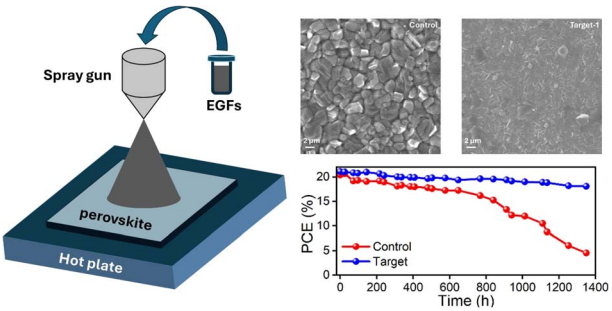
Konstantina Gkini, Spyros Orfanoudakis, Filippos Harlaftis, Panagiotis Dallas, Christos Kouzios, Polychronis Tsipas, Athanassios G. Kontos, Maria Konstantakou and Thomas Stergiopoulos*



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*



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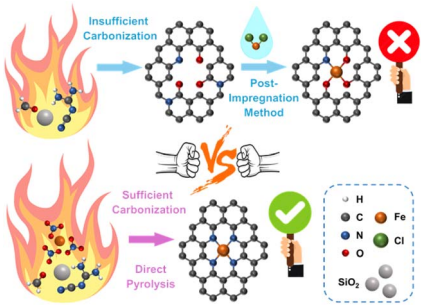
PAPERS

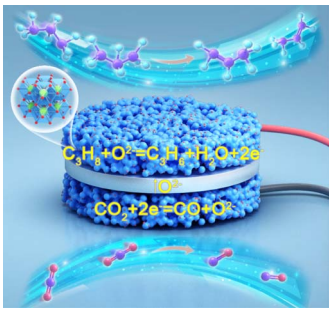
31312



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*

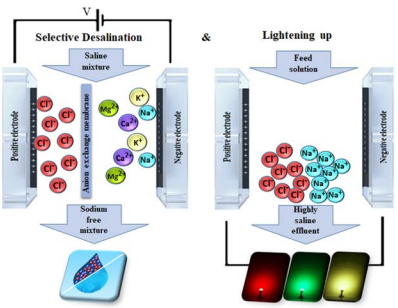
31323



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

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

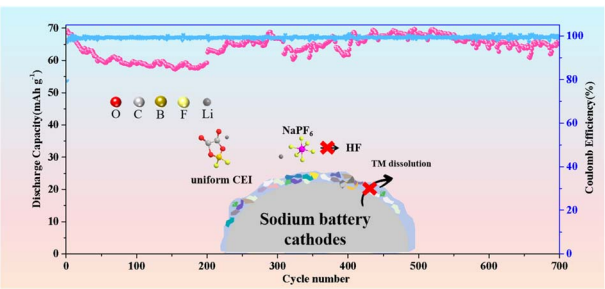
31329



Towards an advanced electrochemical horizon: ion selectivity and energy harnessing through hybrid capacitive deionization with carbon-coated $NaTi_2(PO_4)_3$ and N-rich carbon nests

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

31347



Construction of a stable interface at the $Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$ cathode using LiDFOB electrolyte additives for high-performance sodium-ion batteries

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

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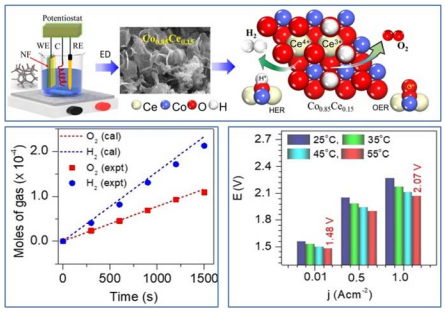
31362

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

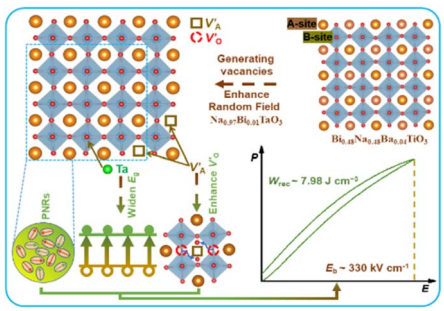
Akbar I. Inamdar,* Amol S. Salunke, Jun Ho Seok, Harish S. Chavan, Nabeen K. Shrestha, Sang Uck Lee,* Sangeun Cho* and Hyunsik Im



31375

Excellent low-field energy storage properties and high density achieved in $Bi_{0.48}Na_{0.48}Ba_{0.04}TiO_3$-based oxide ceramics *via* interposing $(Na_{0.97}Bi_{0.01})^{+}/Ta^{5+}$ at A/B sites

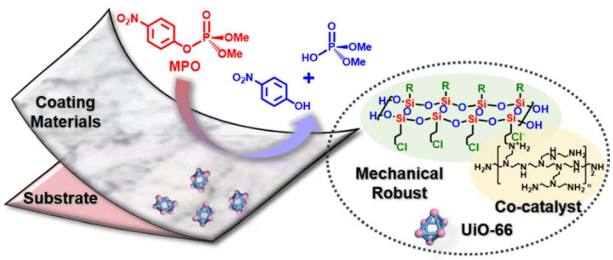
Jiwei Du, Tianhui Shi, Qin Feng,* Ronghao Jia, Jianan Hu, Changlai Yuan,* Xinpeng Wang, Xiyong Chen, Nengneng Luo and Jiwei Zhai*



31386

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

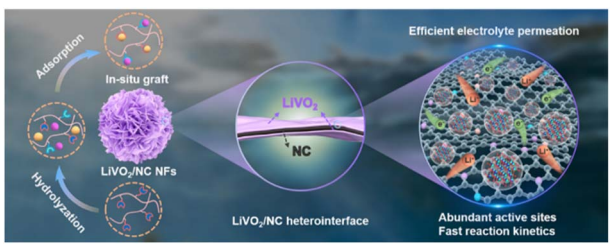
Seungjae Lee, Seungjae Hur, Keunhong Jeong, Hoesun Hwang, Jungkyu Choi, Nithima Khaorapapong, Kyung-Youl Baek, Jin Young Seo,* Yusuke Yamauchi and Jongbeom Na*



31396

Flower-like carbon-confined disordered rock-salt $LiVO_2$ 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*



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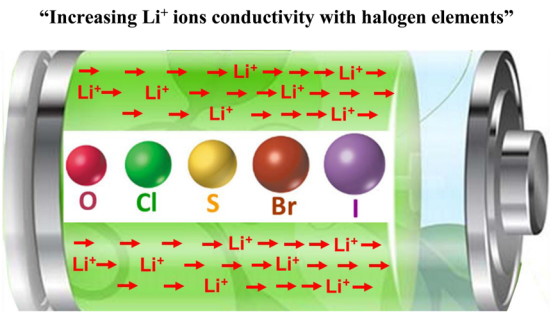
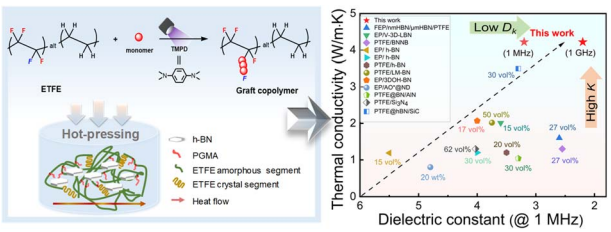


Incorporation of halogens (Cl, Br, and I) in an Li–P–S–O system for exploring new sulfide solid electrolytes with high conductivity and superior electrochemical performance in solid-state batteries

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

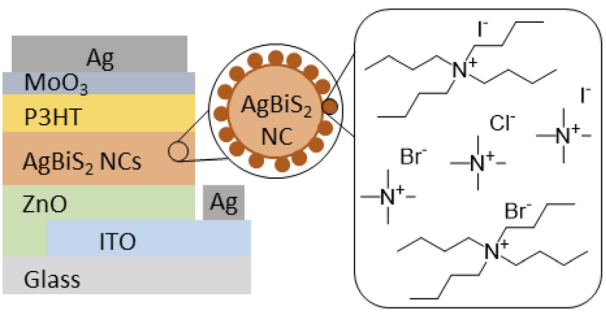
31424



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*

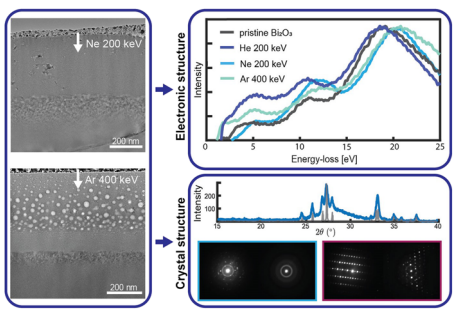
31432



Effect of different halide-based ligands on the passivation and charge carrier dynamics in $AgBiS_2$ 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_2O_3

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

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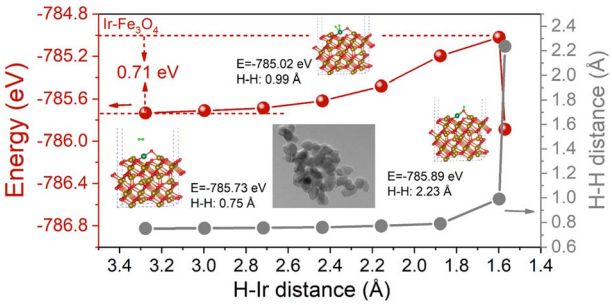
31459

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

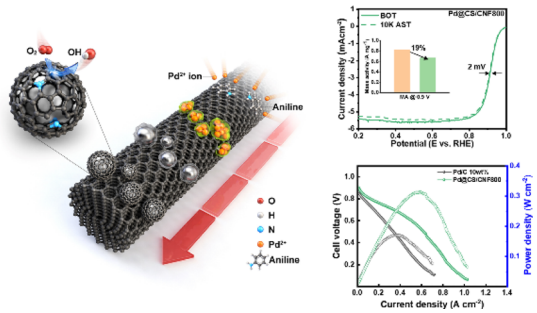
Qiming Tang, Xueling Lei,* Yongliang Zhang, Jiaxin Lu and Kevin Huang*



31467

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

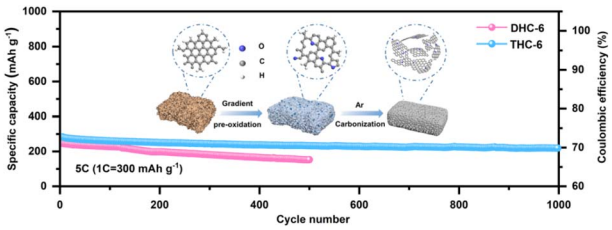
Hyo Eun Bae, Ji Eun Park, T. B. Ngoc Huynh, Jihyeok Song, Sung Ki Cho, Yung-Eun Sung,* Yong-Hun Cho* and Oh Joong Kwon*



31480

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

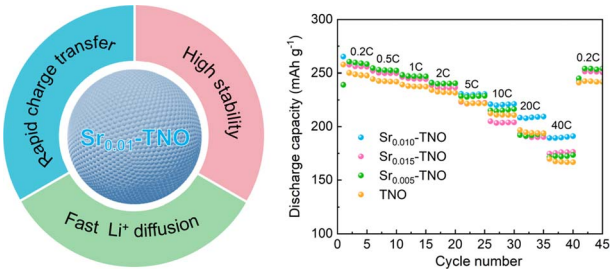
Ling Sheng, Peng Wei, He Ma, Shaoyang Wu, Kang Liang, Jianbin Li,* Qi Wan* and Yurong Ren*



31492

Sr-dopant microstructure engineering enables strong pseudocapacitive effects of $TiNb_2O_7$ 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*



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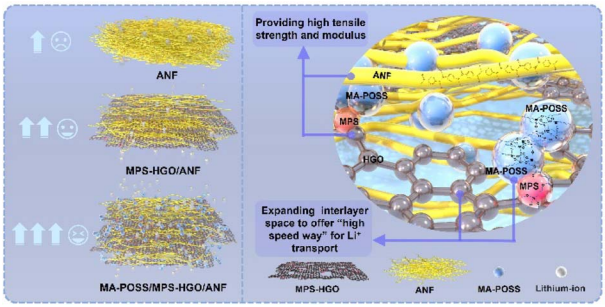
31500



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

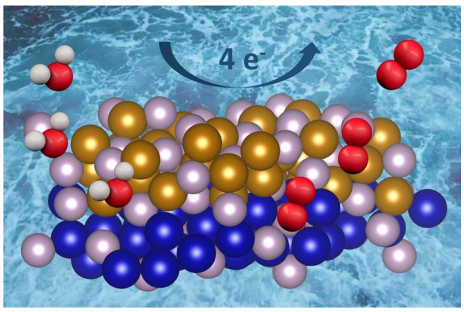
Yuying Wang, Fanjun Guo, Mengzhen Zhou, Qian Wu, Tao You, Zhengxiang Zhong, Jiankun Yang, Li Liu, Yudong Huang* and Mingqiang Wang*

31508

A reversed strategy for designing high-performance anode materials from a traditional $Na_xV_2O_5$ cathode

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

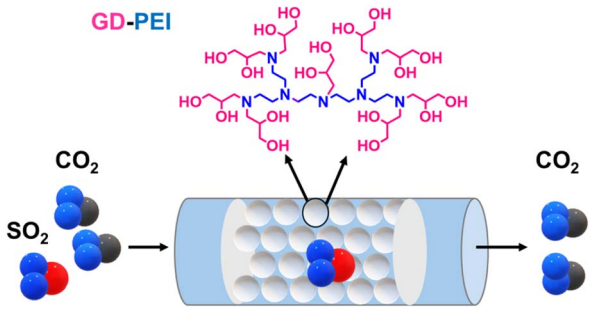
31518



Electron redistribution induced by p–d orbital hybridization in Co_2P/FeP nanosheets boosts water electrooxidation

Qiyan 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 SO_2 in the presence of CO_2

Chanjot Kaur and Abdelhamid Sayari*

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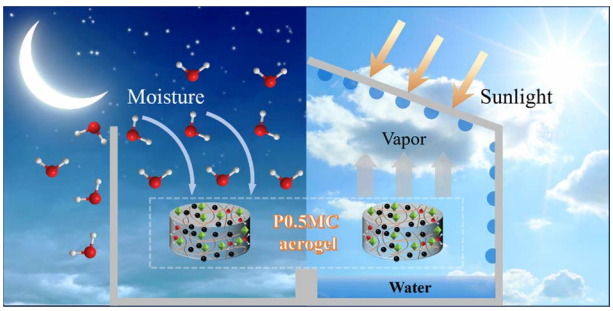
31533

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

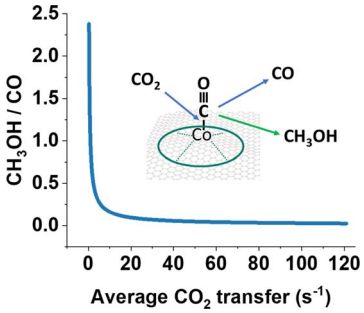
Cai-Hua Liu, Lei Xu,* Zhen-Yu Wang, Sheng-Jie Han, Yi-Bin Li, Ming-Lai Fu* and Baoling Yuan*



31547

Low CO_2 mass transfer promotes methanol and formaldehyde electrosynthesis on cobalt phthalocyanine

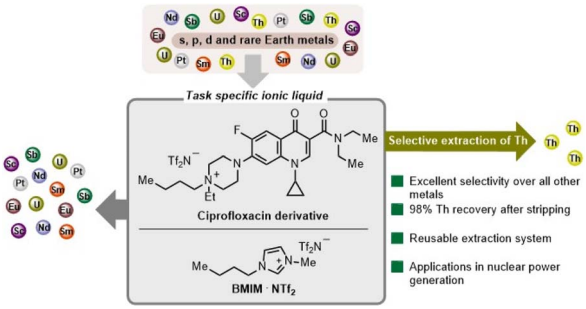
Jie Zhang, Thi Ha My Pham, Shibo Xi, Liping Zhong, David Liem, Futian You, Ben Rowley, Ramesha Ganganahalli, Federico Calle-Vallejo* and Boon Siang Yeo*



31557

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

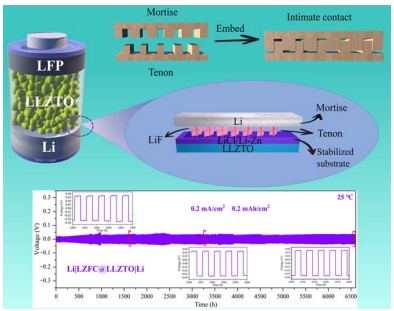
David Lledó, Guillermo Grindlay, H. Q. Nimal Gunaratne, Abel de Cózar, Ana Sirvent and José M. Sansano*



31570

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

Guoxiang Zheng, Yifan Jin, Michal Sedlačík, Elif Vargun, Yifan Zhang, Ying He,* Petr Saha and Qilin Cheng*



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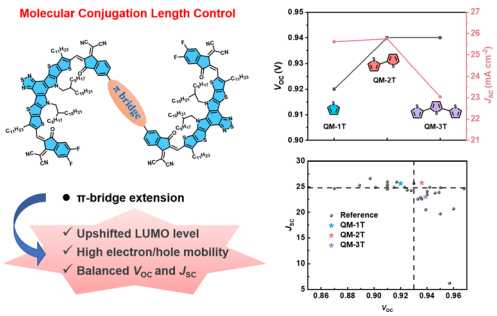
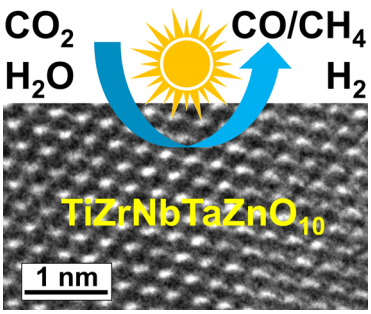
31581



A–π–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

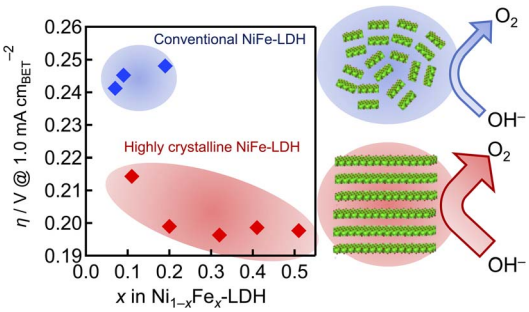
31589



Hybrid d^0 and d^{10} electronic configurations promote photocatalytic activity of high-entropy oxides for CO_2 conversion and water splitting

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

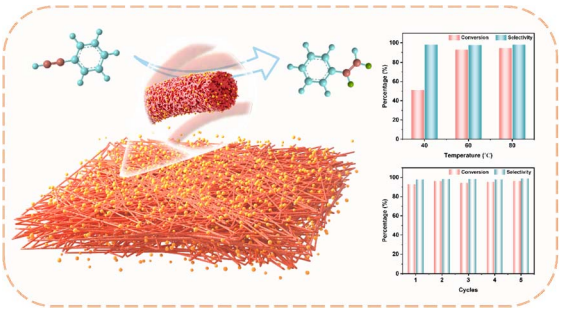
31603



Superior oxygen evolution reaction activities of highly crystalline $Ni_{1-x}Fe_x$-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*

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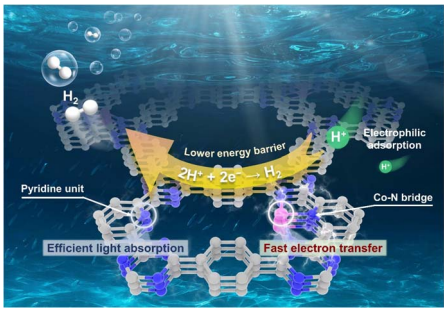
31619

A pyridine-woven covalent organic framework facilitating the immobilization of Co single atoms towards efficient photocatalytic H_2 evolution

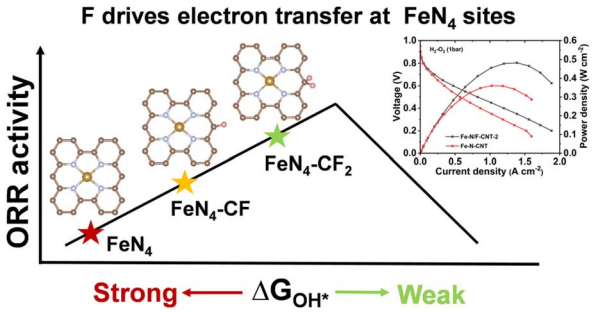
Yanchi Yao, Jingbo Lin, Shasha Liu, Yong Zheng, Lun Lu, Qile Fang, Shuang Song, Chao Zhu* and Yi Shen*



31630

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

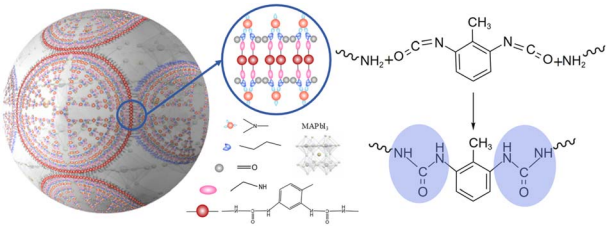
Nan Xue, Jian Yin, Xueyan Xue, Hui Zhu* and Jiao Yin*



31638

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

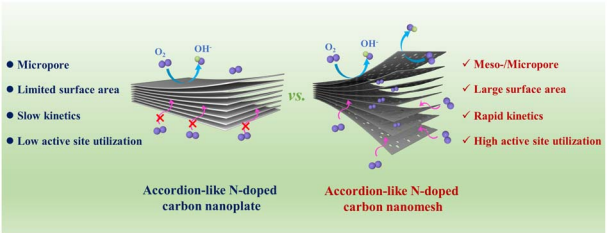
Mengru Liu, Xueqing Ma, Qianyu Zhao, Zhenya Li, Yingliang Liu,* Shengang Xu and Shaokui Cao



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*



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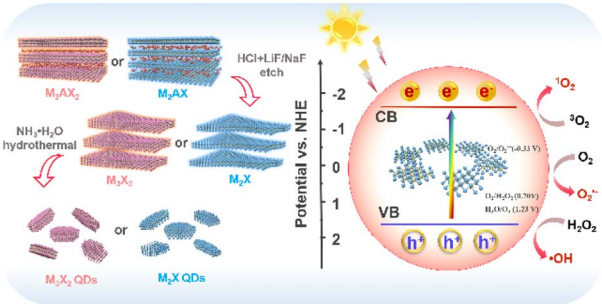

Outstanding ROS generation ability and the mechanism of MXene quantum dots

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

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