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Journal of Materials Chemistry A

Materials for energy and sustainability

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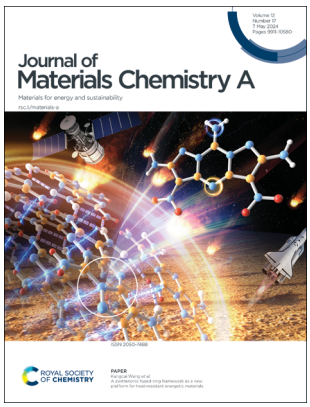
IN THIS ISSUE

ISSN 2050-7488 CODEN JMCAET 12(17) 9911–10580 (2024)



Cover
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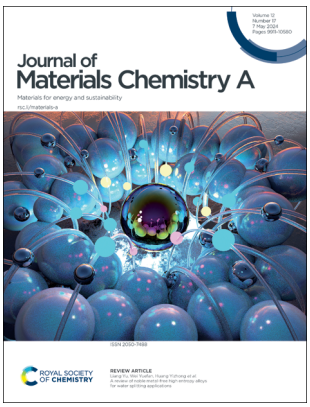


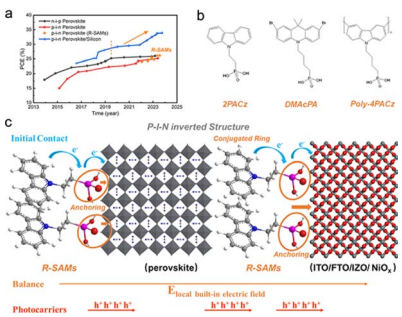
Inside cover
See Liang Yu, Wei Yuefan, Huang Yizhong *et al.*, pp. 9933–9961. Image reproduced by permission of Hamzah Kamaruddin and Huang Yizhong from *J. Mater. Chem. A*, 2024, **12**, 9933.

HIGHLIGHT

9929

Revolutionary SAMs: transforming inverted perovskite solar cells

Hongshi Li* and ShunChang Liu

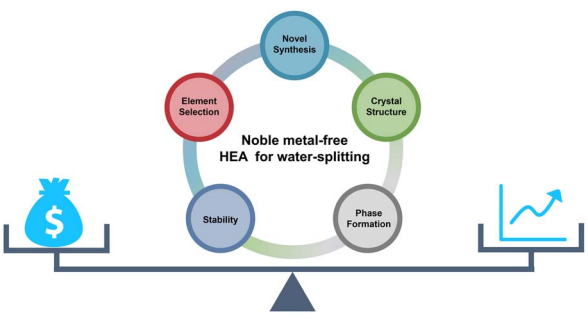


REVIEWS

9933

A review of noble metal-free high entropy alloys for water splitting applications

Hamzah Kamaruddin, Zhang Jianghong, Liang Yu,* Wei Yuefan* and Huang Yizhong*



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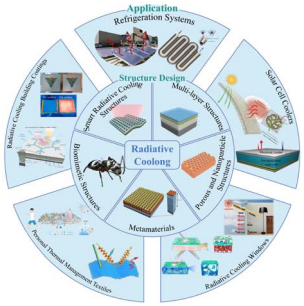
REVIEWS

9962

Radiative cooling: structure design and application

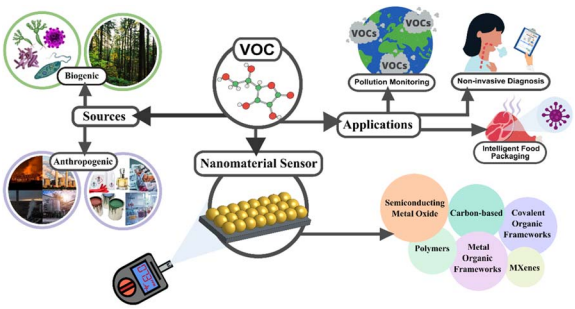
Yi Wang, Haining Ji,* Bin Liu, Pinghua Tang, Yongxing Chen, Jiamei Huang, Yangyong Ou and Jundong Tao



9979

Nanomaterial-based VOC sensing applications and a deep dive into their developmental trends

Warren Rosario, Pravin Kumar Singh, Ashutosh Tiwari, Utkarsh Jain, Devesh Kumar Avasthi and Nidhi Chauhan*



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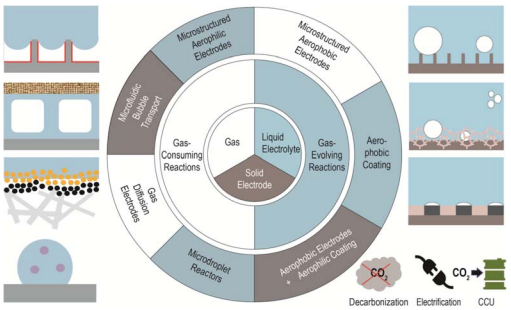
Tailoring hydrophilic and hydrophobic microenvironments for gas–liquid–solid triphase electrochemical reactions

Jungki Ryu* and Dong Woog Lee*

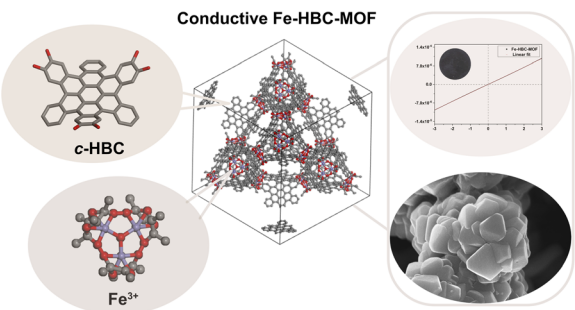


COMMUNICATION

10044

An electrically conducting 3D coronene-based metal–organic framework

Marina I. Schönherr, Patricia I. Scheurle, Laura Frey, Marta Martínez-Abadía, Markus Döblinger, Andre Mähringer, Dominik Fehn, Lena Gerhards, Irina Santourian, Alfred Schirmacher, Tatjana Quast, Gunther Wittstock, Thomas Bein, Karsten Meyer, Aurelio Mateo-Alonso and Dana D. Medina*



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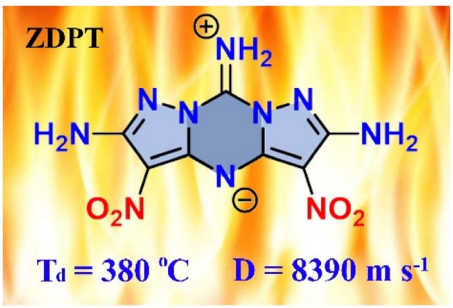
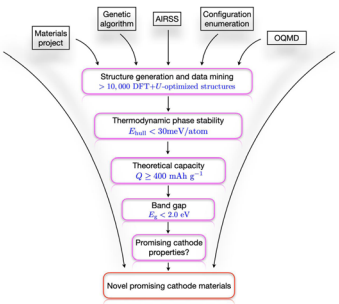
10050



A zwitterionic fused-ring framework as a new platform for heat-resistant energetic materials

Ruibing Lv, Lan Jiang, Jinxin Wang, Shiliang Huang, Siwei Song, Liyuan Wei, Qinghua Zhang and Kangcai Wang*

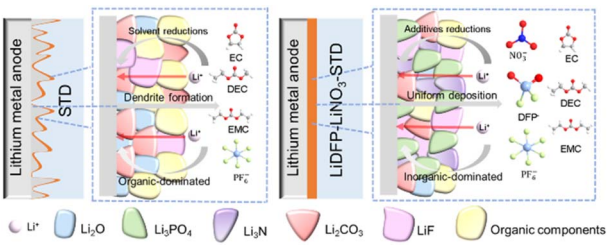
10059



Computational discovery of superior vanadium-niobate-based cathode materials for next-generation all-solid-state lithium-ion battery applications

Tanmoy Chakraborty,* Bartomeu Monserrat, Alexandru Tănase, Richard I. Walton and Bora Karasulu*

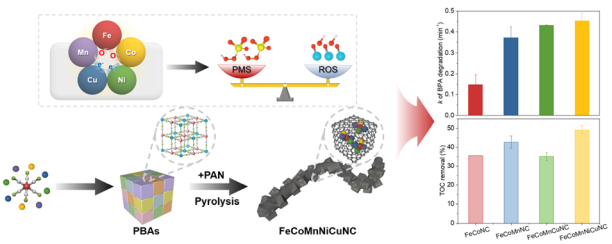
10072



Constructing an inorganic-rich solid electrolyte interphase by adjusting electrolyte additives for stable Li metal anodes

Minghui Li, Cai Chen, Hongze Luo, Qingshuai Xu,* Keyou Yan,* Yongcai Qiu* and Guangmin Zhou

10081



Prussian blue analogue-derived high-entropy alloy nanoarchitectonics for efficient Fenton-like catalysis

Yiyuan Yao, Shifu Wang, Chaohai Wang, Zetong Wu, Chengming Xiao, Xin Guo, Xin Yan, Junwen Qi, Yujun Zhou, Zhigao Zhu, Yue Yang, Xuning Li and Jiansheng Li*

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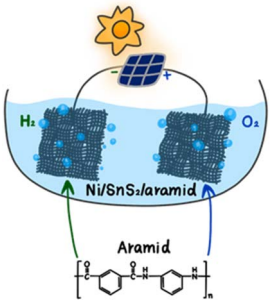
10090

A low-cost and large-area modular nickel electrode on aramid fabric for efficient solar-driven water electrolysis

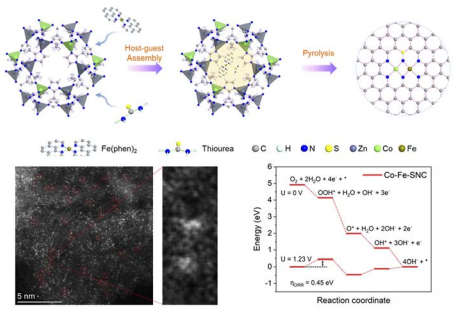
Yuling Yuan, Zhiping Mao, Hong Xu,* Fatwa F. Abdi* and Yimeng Ma*



10101

Design of S, N-codoped Co–Fe dual-atom sites for efficient alkaline oxygen reduction

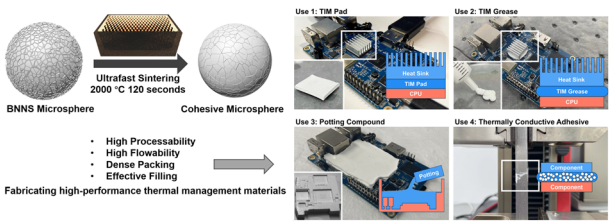
Ning He, Yuanmiao Sun, Xiaoyang Chen, Jiaqi Wang, Guojin Liang* and Funian Mo*



10110

Ultrafast sintering of boron nitride nanosheet assembled microspheres with strong processability for high-performance thermal management materials

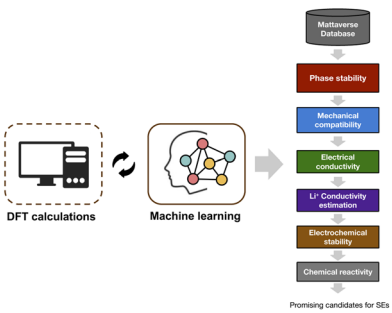
Siyuan Ding, Fangzheng Zhen, Yu Du, Ke Zhan, Yinghui Wu, Jiuyi Zhu, Qijun Zheng, Baofu Ding, Aibing Yu, Hui-Ming Cheng, Minsu Liu* and Ling Qiu*



10124

Machine-learning assisted high-throughput discovery of solid-state electrolytes for Li-ion batteries

Xingyu Guo,* Zhenbin Wang, Ji-Hui Yang and Xin-Gao Gong*



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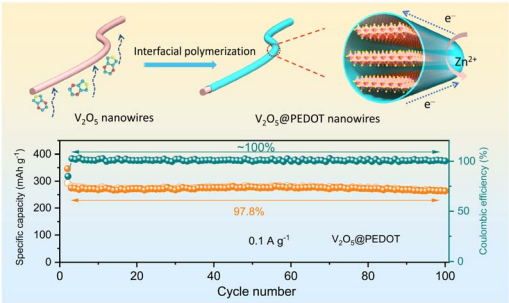
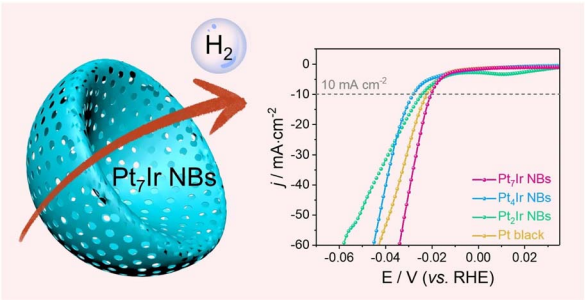


Interfacial polymerization of PEDOT sheath on V_2O_5 nanowires for stable aqueous zinc ion storage

Ting Yang, Diheng Xin, Nan Zhang, Jing Li, Xianchi Zhang, Liqin Dang, Qi Li, Jie Sun, Xuexia He, Ruibin Jiang, Zonghuai Liu and Zhibin Lei*

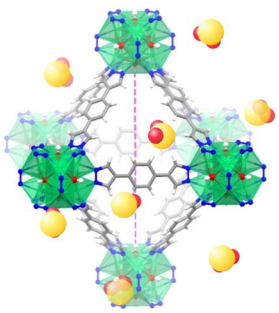
10148



Engineering ultrafine PtIr alloy nanoparticles into porous nanobowls *via* a reactive template-engaged assembly strategy for high-performance electrocatalytic hydrogen production

Zhenbo Zhang, Shuyun Liu, Yudie Zhou, Jing Li, Lin Xu,* Jun Yang,* Huan Pang, Mingyi Zhang and Yawen Tang*

10157



Impact of Ni(II) coordinatively unsaturated sites and coordinated water molecules on SO_2 adsorption by a MOF with octanuclear metal clusters

Juan L. Obeso, Karuppasamy Gopalsamy, Mohammad Wahiduzzaman, Eva Martínez-Ahumada, Dong Fan, Hugo A. Lara-García, Francisco J. Carmona, Guillaume Maurin,* Ilich A. Ibarra* and Jorge A. R. Navarro*

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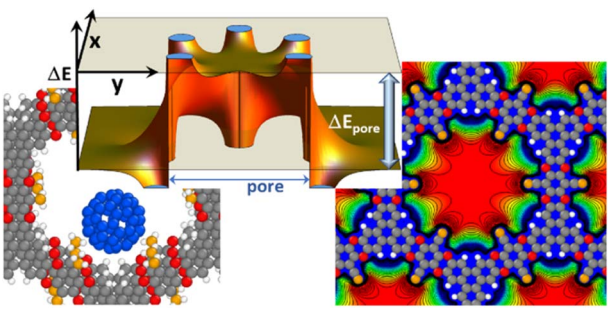

Tuning the electrostatic energy landscape within the pores of covalent organic frameworks: post-synthetic modification reactions and structural imperfections

Egbert Zojer

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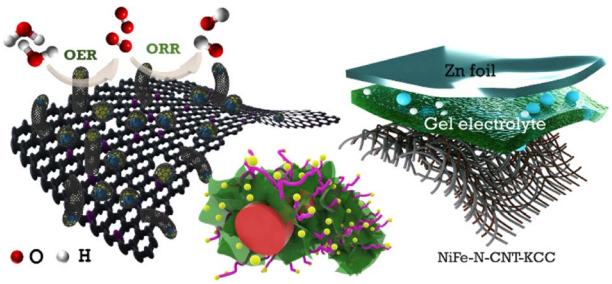
Pyridinic-N exclusively enriched CNT-encapsulated NiFe interfacial alloy nanoparticles on knitted carbon fiber cloth as bifunctional oxygen catalysts for biaxially flexible zinc–air batteries

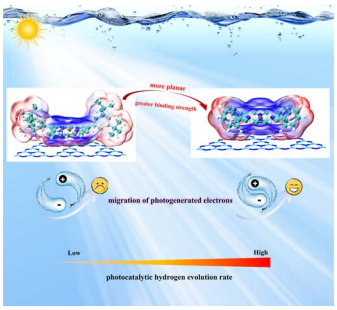
Milan Babu Poudel, Subramanian Vijayapradeep, Karthikeyan Sekar, Jong Seok Kim and Dong Jin Yoo*



10196

Molecular conformation: a key factor underlying the performances of heterojunction photocatalysts

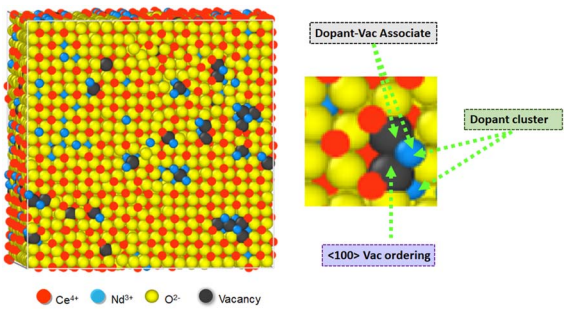
Wanyu Liang, Ruyue Jiang, Xiao Tian, Hantang Zhang,* Bowen Zhang,* Xiuqiang Lu,* Jie Liu, Lang Jiang, Shifeng Hou and Shiyun Ai



10203

Dopant clustering and vacancy ordering in neodymium doped ceria

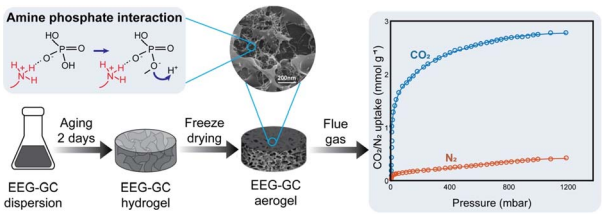
Jing Ming, Marzena Leszczyńska-Redek,* Marcin Malys, Wojciech Wrobel, Jan Jamroz, Michal Struzik, Stephen Hull, Franciszek Krok and Isaac Abrahams*



10216

Sustainable CO_2 adsorbent *via* amine–phosphate coupling of glycated chitosan and electrochemically exfoliated graphene

Sucharita Pal, Edward P. L. Roberts, Milana Trifkovic* and Giovanniantonio Natale*



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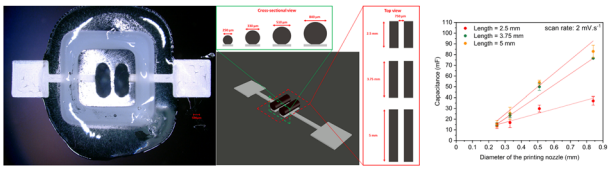
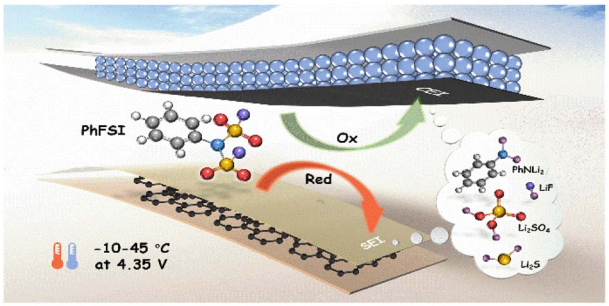


Scaling of 3D-printed microsupercapacitors to mm³ volumes.

Sub-mm³ dimensional scaling of fully-integrated additively-fabricated microsupercapacitors for embedded energy storage applications

Amin Hodaei and Vivek Subramanian*

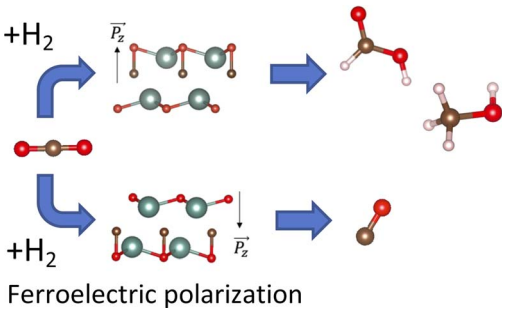
10242



A straightforward approach to improve NCM523/graphite pouch battery performance in a wide temperature range at 4.35 V using film-forming additive *N*-phenylimidodisulfuryl fluoride (PhFSI)

Guoliang Yang, Zhaohao Huang, Irfan Majeed, Chaojun Fan, Jiasheng Lu, Kai Wang, Weizhen Fan,* Jingwei Zhao* and Zhuo Zeng*

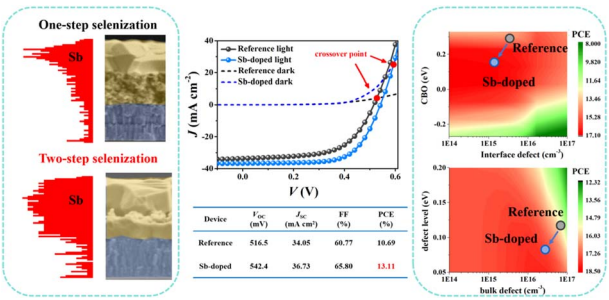
10252



***Ab initio* investigation of tunable CO_2 reduction reaction on the two dimensional ferroelectric Y_2CO_2**

Mo Li and Joshua Young*

10260



Device	V_{oc} (mV)	J_{sc} (mA cm²)	FF (%)	PCE (%)
Reference	516.5	34.05	60.77	10.69
Sb-doped	542.4	36.73	65.80	13.11

Defect-level trap optimization in $Cu_2ZnSn(S,Se)_4$ photovoltaic materials *via* Sb^{3+}-doping for over 13% efficiency solar cells

Yingfen Li, Xingye Chen,* Runxi Wang, Nian Zhou, Fang Huang, Jun Zhao,* Zhenghua Su, Shuo Chen and Guangxing Liang*

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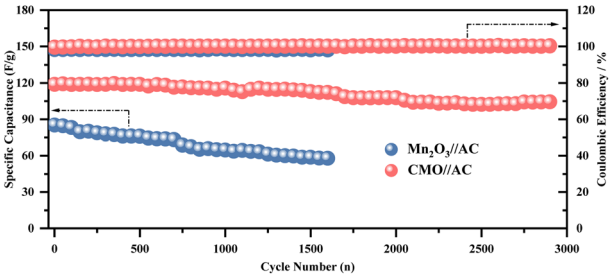
PAPERS

10269

Trace Cs induced phase transition of Mn_2O_3 for enhanced magnesium ion capacitors

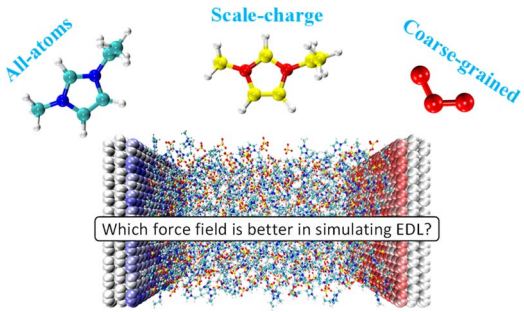
Mudi Li, Yaxi Ding, Siwen Zhang,* Minghui Liu, Ying Sun, Yusheng Zhang, Bosi Yin* and Tianyi Ma*



10279

Accurately simulating electrical double layers structure and formation using all-atom scaled-charge force fields

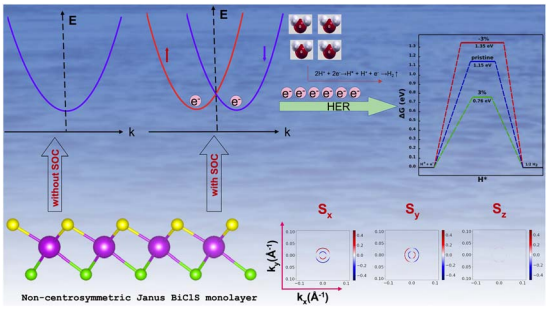
Haoyu He, Jianguo Zhou, Lei Yang, Chenglin Liang, Shuaikai Xu, Ming Chen and Tangming Mo*



10287

Establishing the correlation between Rashba spin splitting and HER activity enhancement in Janus structures

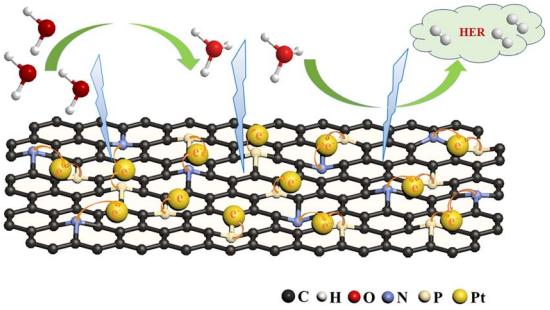
Dhirendra Kumar and Sudip Chakraborty*



10300

N, P co-doped graphene-supported monometallic nanoparticles for highly efficient hydrogen evolution by acid electrolysis of water

Fengshun Wu, Li Zeng, An Pei, Yingliang Feng and Lihua Zhu*



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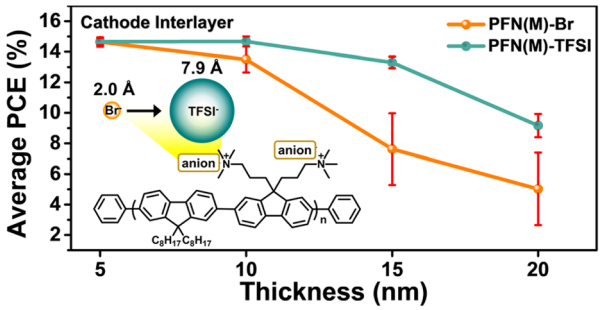
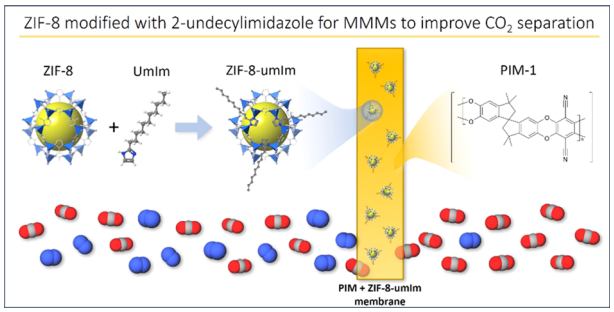


Counter-anion size engineering in polyfluorene-based cathode interlayers to enhance thickness independence

Yurim Bae, Jeongsu Kim, Sang Ah Park, Haeryang Lim, Dae Hwan Lee, Taiho Park* and Yelim Choi*

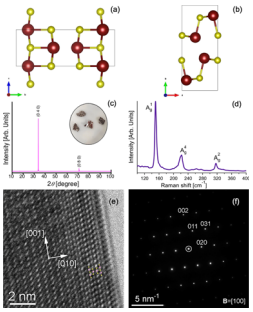
10316



ZIF-8 modified with 2-undecylimidazolate as filler for mixed matrix membranes for CO_2 separation

Marta Pérez-Miana, José Miguel Luque-Alled, Mohamed Yahia, Álvaro Mayoral and Joaquín Coronas*

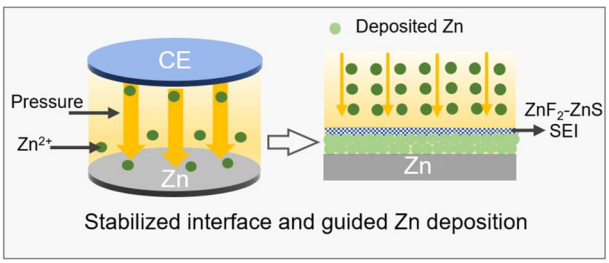
10329



Unlocking superior NO_2 sensitivity and selectivity: the role of sulfur abstraction in indium sulfide (InS) nanosheet-based sensors

Gianluca D'Olimpio, Danil W. Boukhvalov,* Vardan Galstyan, Jessica Occhiuzzi, Michael Vorochta, Matteo Amati, Zygmunt Milosz, Luca Gregoratti, Marian Cosmin Istrate, Chia-Nung Kuo, Chin Shan Lue, Corneliu Ghica, Elisabetta Comini and Antonio Politano*

10341



Guiding uniform Zn electrodeposition through regulating pressure for stable aqueous Zn batteries

Fenglin Zhang, Ziyang Cai, Runtao Liu, Yang Sun and Huilin Pan*

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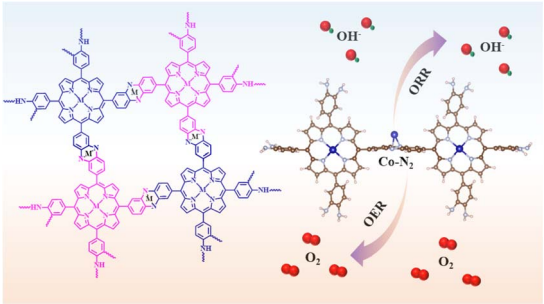
10349

Microcosmic modulation of the Co–N bonding structure improves the multi-functional electrocatalytic performance

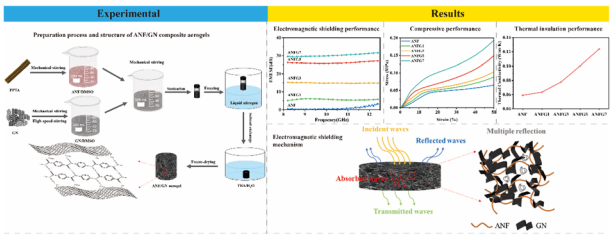
Wenhui Deng, Tianjing Wu,* Yufeng Wu, Fang Chen, Yansong Bai, Xiaoqing Zou, Mingjun Jing,* Wentao Deng, Hongshuai Hou and Xianyou Wang



10359

Electromagnetic interference shielding performance of lightweight aramid nanofiber/graphene composite aerogels

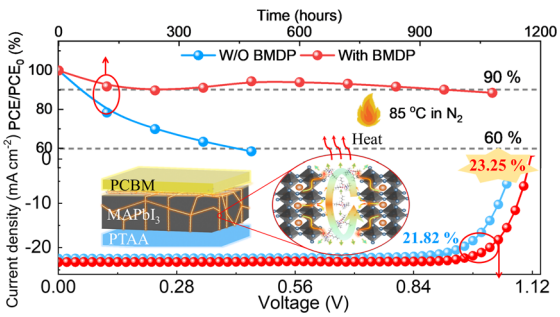
Nian Luo, Yi-yin Zhang, Huan Zhang, Ting-long Liu, Yu Wang, Feng Chen* and Qiang Fu*



10369

Multi-functional thermal management for efficient and stable inverted perovskite solar cells

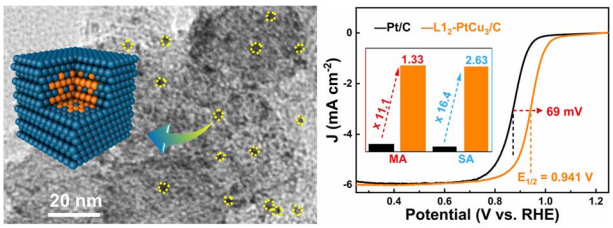
Yongsong Zhang, Zhen He, Jian Xiong,* Shiping Zhan, Fu Liu, Meng Su, Dongjie Wang, Yu Huang, Qiaogan Liao, Jiangrong Lu, Zheling Zhang, Changlai Yuan, Jiang Wang, Qilin Dai* and Jian Zhang*



10385

A sub-4 nm $PtCu_3$ intermetallic catalyst with an $L1_2$-ordered structure toward efficient activity and durability for oxygen reduction

Haibo Jiang, Xiang Xie, Liyuan Bi, Shengwei Yu, Jiaxi Zeng, Lili Zhang, Jianhua Shen* and Chunzhong Li*



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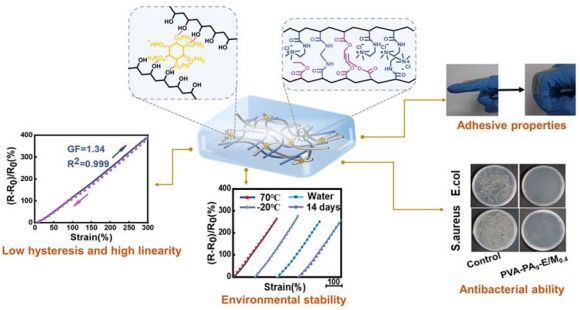
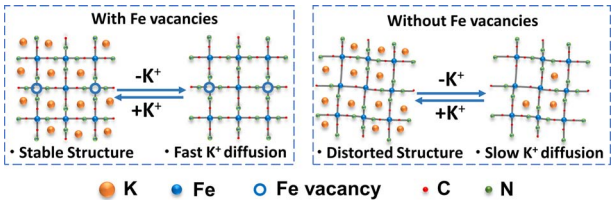
10392



Low-hysteresis and highly linear sensors based on environmentally stable, adhesive, and antibacterial hydrogels

Chengmeng Wei, Yao Wang, Yongjie Liang, Jiaming Wu, Feng Li, Qiuxia Luo, Yewei Lu, Cuiwen Liu, Ru Zhang, Zhenpin Lu, Baiping Xu, Ning Qing* and Liuyan Tang*

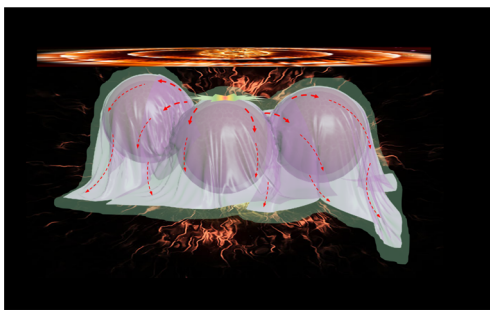
10403



Fe^{HS} vacancies in a Prussian white cathode leads to enhanced Fe^{LS} activity and electrode kinetics for boosted K^+ storage

Shun Zi, Zixing Wang, Jinlong Ke, Ying Mo, Kexuan Wang, Shi Chen, Rui Tang,* Yanhua Li,* Peng Gao* and Jilei Liu

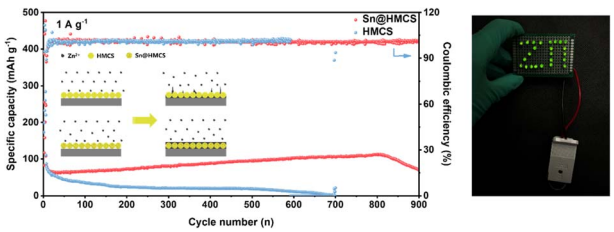
10412



Flexible-rigid covalent nano-template of micron porous silicon towards ultra-robust Li-ion batteries

Baoping Liu, HanJiang Li, Wen Luo,* Xiaofeng Zhang,* Zhongyun Liu, Pengfei Yin and Rui Zhang*

10422



Controllable synthesis of an atomic Sn-anchoring carbon host for excellent long-cycle-life zinc metal batteries

Lantao Liu, Yiming Li, Hu Zhang, Fang Dong, Shuaize Wang, Ziyu Sun, Gaixia Zhang,* Xiaohong Chen,* Sasha Omanovic, Shuhui Sun* and Huaihe Song*

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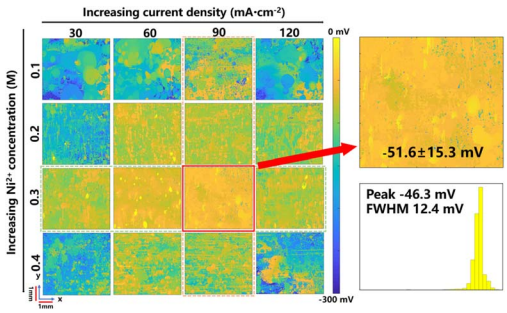
10429

Optimization of a NiMo catalytic electrode based on the distribution map of HER onset potential

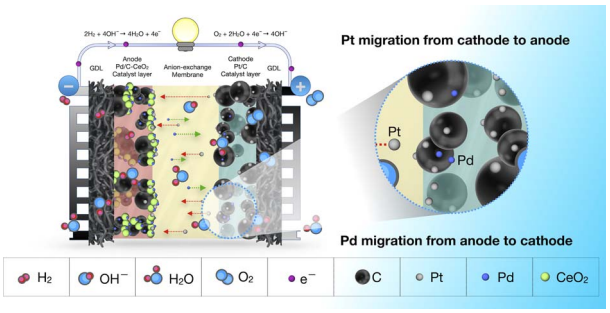
Xuyang Ma, Jiqiang Dong, Fuying Li, Kaijie Ma, Le Liu* and Jingyu Xi*



10435

Elucidating the degradation mechanisms of Pt-free anode anion-exchange membrane fuel cells after durability testing

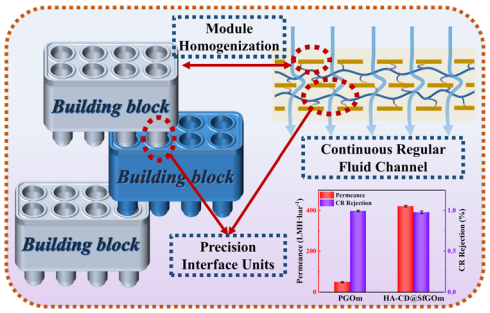
John C. Douglin, Ramesh K. Singh, Ami C. Yang-Neyerlin, Cheng He, Karam Yassin, Hamish A. Miller, Maria V. Pagliaro, Laura Capozzoli, Enrique Carbo-Argibay, Simon Brandon, Paulo J. Ferreira, Bryan S. Pivovar* and Dario R. Dekel*



10449

LEGO® brick-inspired ultra-stable and rapid transport 2D membrane for fast water purification

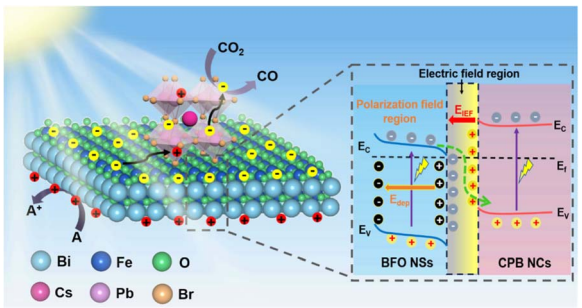
Bo Zhu, Nan Li,* Changsheng Guo, Pengbi Liu, Tianyu Li, Lijing Wang and Zhiwei Xu*



10461

Enhancing photocatalytic CO_2 reduction *via* a single-domain ferroelectric Z-scheme heterojunction of $BiFeO_3/CsPbBr_3$ inducing dual built-in electric fields

Danrui Pan, Yi Lu, Ahmed Mahmoud Idris,* Zhihao Chen, Leyi Xu, Jin Wang, Guocan Jiang, Zhaojiang Chen* and Zhengquan Li*



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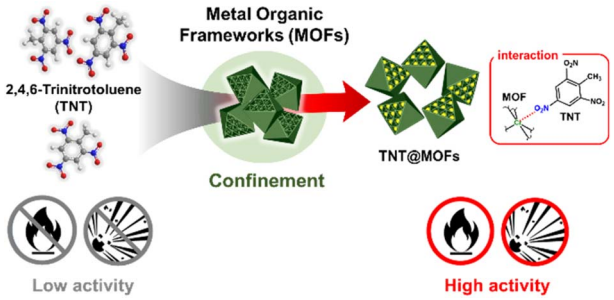
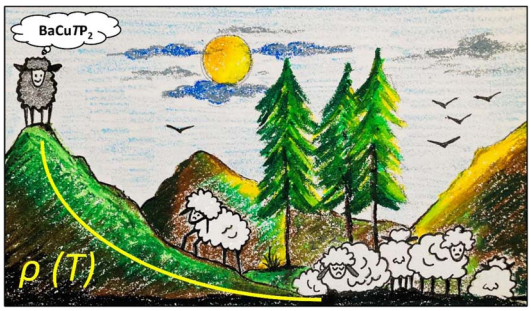
10472



Facilitated explosion of nitro compounds confined in metal–organic frameworks

Eun-Young Kim, Mingu Han, Seong Han Kim, Hye Jung Joe, Seok Ki Kim,* Youn-Sang Bae* and Su-Young Moon*

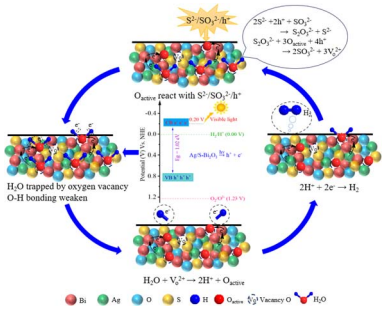
10481



BaCuTP$_2$ (T = Al, Ga, In): a semiconducting black sheep in the ThCr$_2$Si$_2$ intermetallic family

Arka Sarkar, Andrew P. Porter, Gayatri Viswanathan, Philip Yox, Rae Ann Earnest, Jian Wang, Aaron J. Rossini and Kirill Kovnir*

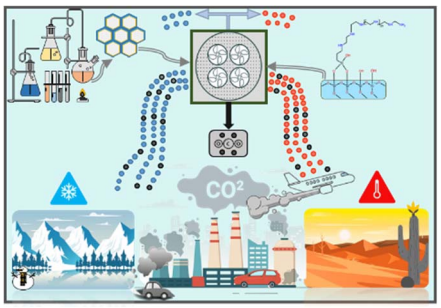
10494



Synergistic vacancy defects and bandgap engineering in an Ag/S co-doped Bi$_2$O$_3$-based sulfur oxide catalyst for efficient hydrogen evolution

Zhengjie Su, Xinru Wu, Dong-Hau Kuo,* Baoqian Yang, Binghong Wu, Longyan Chen, Pengkun Zhang, Jinguo Lin,* Dongfang Lu* and Xiaoyun Chen*

10507



Ambient and sub-ambient temperature direct air CO$_2$ capture (DAC) by novel supported *in situ* polymerized amines

Akram A. Al-Absi, Anne M. Benneker and Nader Mahinpey*

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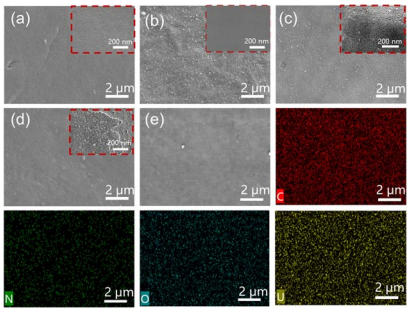
10528

Hydrazide and amidoxime dual functional membranes for uranium extraction from seawater

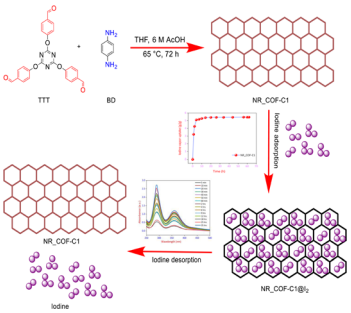
Yunyou Yao, Jian Liao, Xiao Xu, Chen Huang, Mengtao Fu, Kang Chen, Lin Ma, Jiaguang Han, Lu Xu* and Hongjuan Ma*



10539

Facile synthesis of a nitrogen-rich covalent organic framework for the efficient capture of iodine

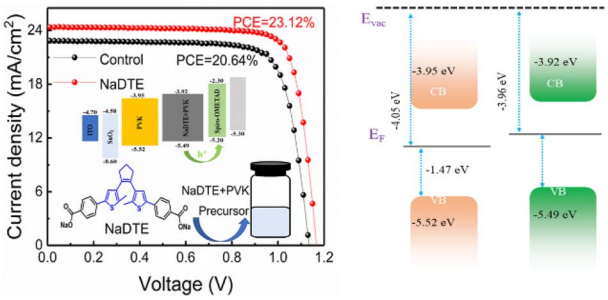
Nowsheenah Farooq, Abu Taha and Athar Adil Hashmi*



10554

A simple passivation strategy of Na-dithienylethene for highly efficient and stable perovskite solar cells

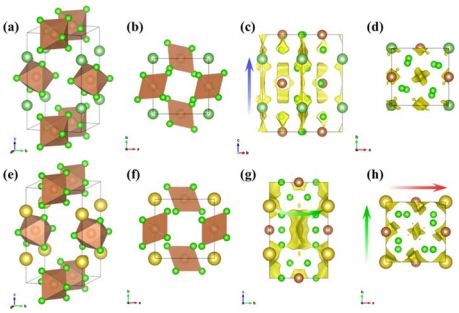
Xianhu Wu, Nian Liu, Guiyuan Wu,* Guanglei Cui,* Rumeng Shi, Gaojie Xia, Jieyu Bi, Haidong Huang, Chunyi Zhao, Zewen Zuo and Min Gu

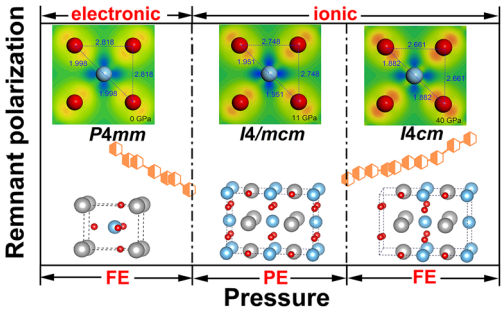


10562

First-principles study on a new chloride solid lithium-ion conductor material with high ionic conductivity

Xiao Fu, Yuqi Wang, Jing Xu, Qifan Yang, Huican Mao,* Ruijuan Xiao* and Hong Li





Pressure-induced electronic to ionic phase transition and recurrence of ferroelectricity in $PbTiO_3$

Xin Zhang, Caoyuan Mu, Yonghao Han, Xue Liu, Hao Liu, Dawei Jiang, Muyun Han, Jia Wang* and Lin Zhao*

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