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Journal of Materials Chemistry A

Materials for energy and sustainability

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IN THIS ISSUE

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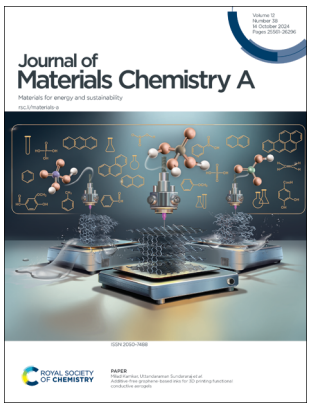

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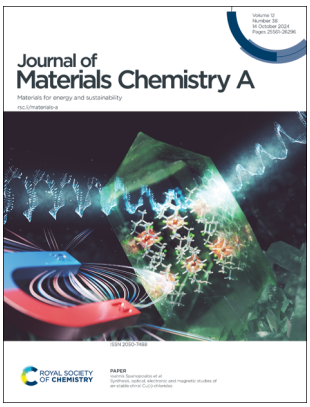

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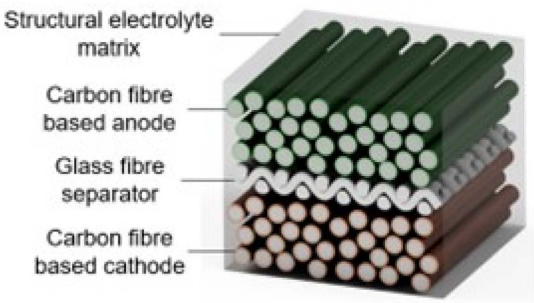
REVIEWS

25580

Carbon fibre based electrodes for structural batteries

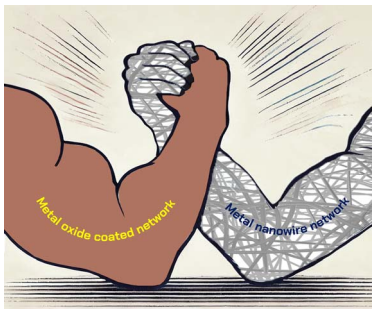
Rob Gray,* Thomas Barthelay,* Chris R. Bowen, Frank Marken, Alexander J. G. Lunt, Leif E. Asp, Dan Zenkert, Paloma Santana Rodriguez, Johanna Xu, Karl Bouton and Andrew T. Rhead*



25600

Towards enhanced transparent conductive nanocomposites based on metallic nanowire networks coated with metal oxides: a brief review

Abderrahime Sekkat,* Camilo Sanchez-Velasquez, Laetitia Bardet, Matthieu Weber, Carmen Jiménez, Daniel Bellet, David Muñoz-Rojas* and Viet Huong Nguyen*



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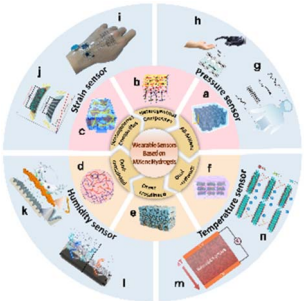
REVIEWS

25622

Toward next-generation wearable sensors based on MXene hydrogels

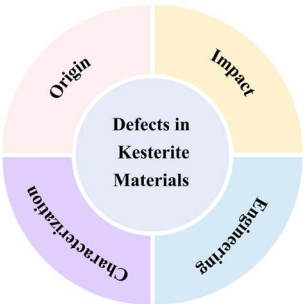
Qinglong He, Chendong Zhao, Hao Chen, Tianzhao Wu, Chuijin Zeng, Yiwen Chen and Chuanfang Zhang*



25643

Defects in kesterite materials towards high-efficiency solar cells: origin, impact, characterization, and engineering

Lijing Wang, Jintang Ban, Litao Han,* Zhengji Zhou, Wenhui Zhou, Dongxing Kou, Yuena Meng, Yafang Qi, Shengjie Yuan and Sixin Wu*



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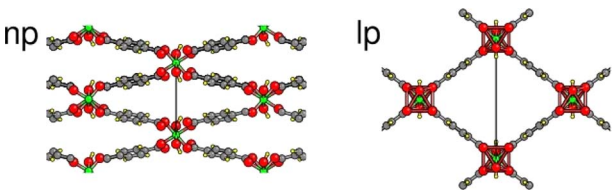
Integrating crystallographic and computational approaches to carbon-capture materials for the mitigation of climate change

Eric Cockayne,* Austin McDannald, Winnie Wong-Ng, Yu-Sheng Chen, Jason Benedict, Felipe Gándara Barragán, Christopher H. Hendon, David A. Keen, Ute Kolb, Lan Li, Shengqian Ma, William Morris, Aditya Nandy, Tomče Runčevski, Mustapha Soukri, Anuroop Sriram, Janice A. Steckel, John Findley, Chris Wilmer, Taner Yildirim, Wei Zhou, Igor Levin and Craig Brown



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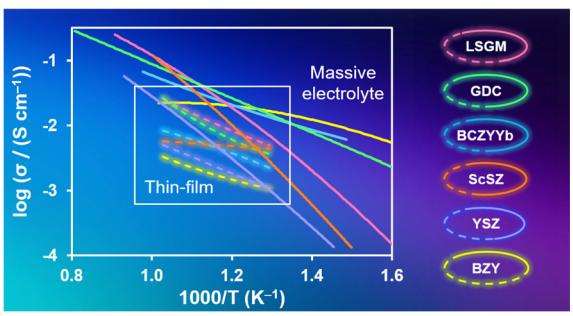
Revisiting the ionic conductivity of solid oxide electrolytes: a technical review

Danil E. Matkin, Inna A. Starostina,* Muhammad Bilal Hanif and Dmitry A. Medvedev*



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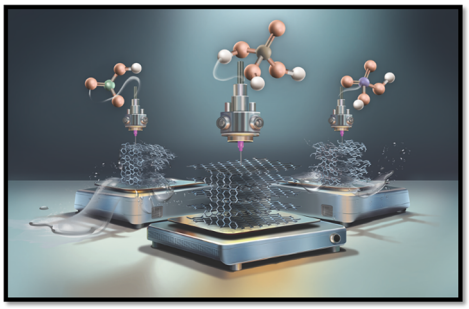
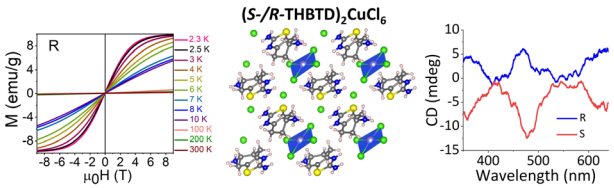


Additive-free graphene-based inks for 3D printing functional conductive aerogels

Elnaz Erfanian, Milad Goodarzi, Gabriel Banvillet, Farbod Sharif, Mohammad Arjmand, Orlando J. Rojas, Milad Kamkar* and Uttandaraman Sundararaj*

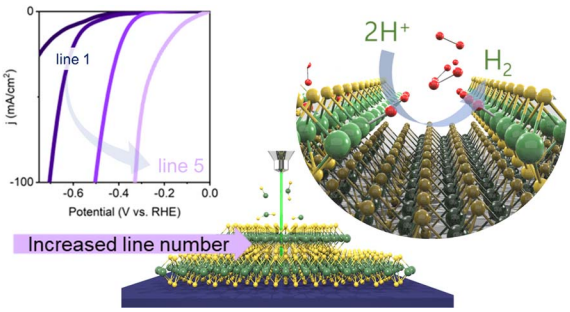
25730



Synthesis, optical, electronic and magnetic studies of air-stable chiral Cu(II) chlorides

Ali Azmy, Nivarthana W. Y. A. Y. Mudiyanselage, Kamal E. S. Nassar, Mike Pham, Nourdine Zibouche, Manh-Huong Phan and Ioannis Spanopoulos*

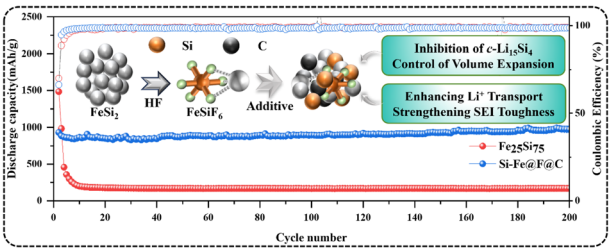
25740



Path-dependent hydrogen evolution reaction *via* selective etching of bilayer MoS_2 catalysts

Min Jung, Jungmoon Lim, Junsung Byeon, Taehun Kim, Younghoon Lim, Hongju Park, Jaesik Eom, Seungsub Lee, Sangyeon Pak* and SeungNam Cha*

25747



Mitigating the volume expansion and enhancing the cycling stability of ferrous fluorosilicate-modified silicon-based composite anodes for lithium-ion batteries

Jichang Sun, Xiaoyi Liu, Penglun Zheng,* Yang Zhao, Yun Zheng,* Jingchao Chai and Zhihong Liu*

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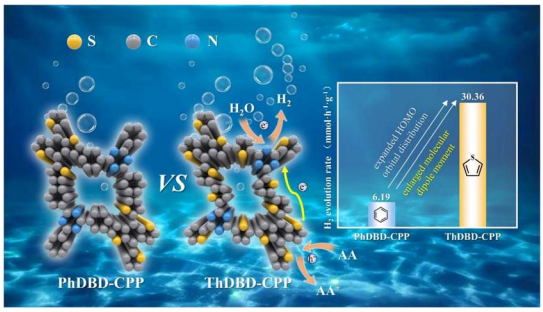
25761

Cross-linked conjugated polymers based on triazine and polybranched polycyclic thiophene for improved photocatalytic hydrogen evolution

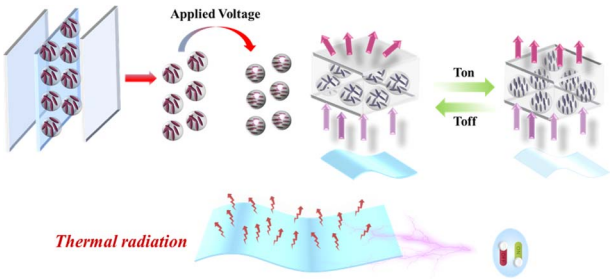
Zibin Li, Ya Chu, Fanpeng Meng, YunYun Dong, Jinsheng Zhao,* Huayang Zhang* and Xiujuan Zhong*



25773

An intelligent electrochromic film with passive radiative cooling and synergistic solar light control capabilities for displays and smart windows

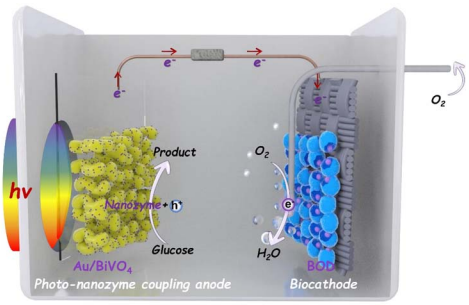
Zuowei Zhang, Xian He, Meina Yu,* Luoning Zhang, Xiao Xiao, Cheng Zou, Yanzi Gao, Qian Wang* and Huai Yang*



25784

Photo-nanozyme coupling catalyzes glucose oxidation for high-performance enzymatic biofuel cells

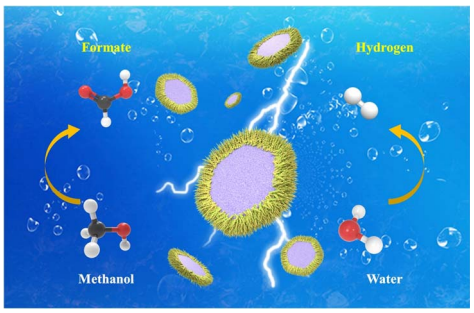
Dandan Hu, Qiwen Su, Yan Gao, Jian-Rong Zhang,* Linlin Wang* and Jun-Jie Zhu*



25791

An efficient $NiCoSe_4$/NiCo-LDH/CF catalyst for the co-production of value-added formate and hydrogen *via* selective methanol electro-oxidation

Jiaxin Li, Hongmei Yu,* Jun Chi, Xu Luo, Tongzhou Li and Zhigang Shao



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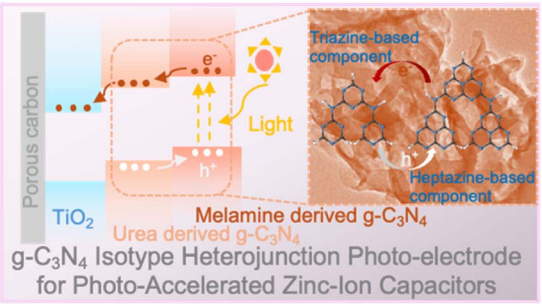

Isotype heterojunction graphitic carbon nitride photocathode for photo-accelerated zinc-ion capacitors

Xiaopeng Liu, Yijia Zhu, Firoz Alam, Tianlei Wang, Ivan P. Parkin, Mingqing Wang and Buddha Deka Boruah*

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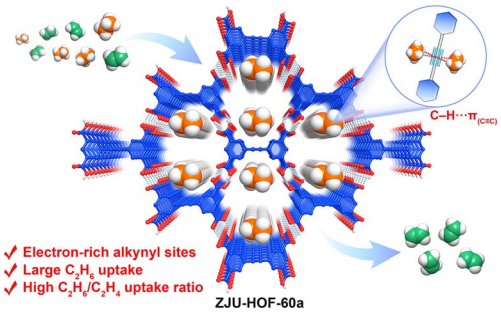
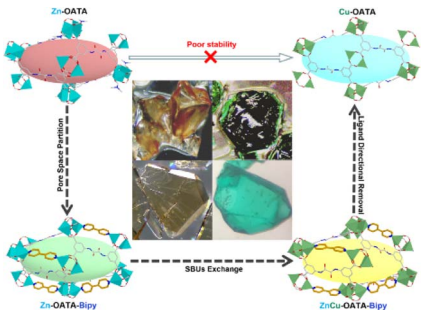


A novel microporous hydrogen-bonded organic framework with electron-rich alkynyl groups for highly efficient C_2H_6/C_2H_4 separation

Yu-Bo Wang, Teng-Fei Zhang, Yu-Xin Lin, Jia-Xin Wang, Hui-Min Wen, Xu Zhang,* Guodong Qian and Bin Li*

25820



Creating a MOF with larger pores and higher stability for gas separation through continuous structure transformation

Lin Zhang, Gang-Ding Wang, Bin Zhang, Guo-Ping Yang, Wen-Yan Zhang, Lei Hou,* Yao-Yu Wang and Zhonghua Zhu

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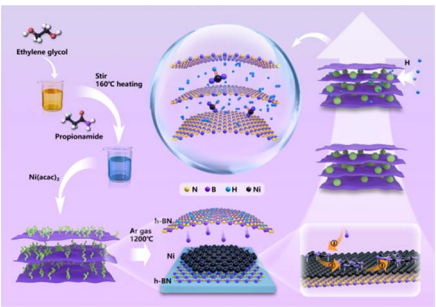

***In situ* construction of dual-functional Ni/Ni_xB catalysts for the hydrogenation and dehydrogenation of magnesium hydride**

Hui Liang,* Wenjiang Li and Jie Zheng*

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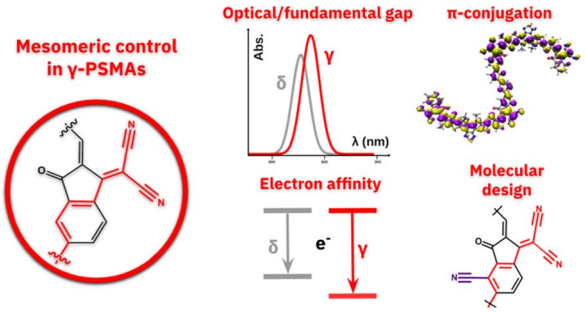
Mesomeric control of the optoelectronic properties of polymerized small molecule acceptors

Diego Sorbelli, Yilei Wu, Zhenan Bao and Giulia Galli*



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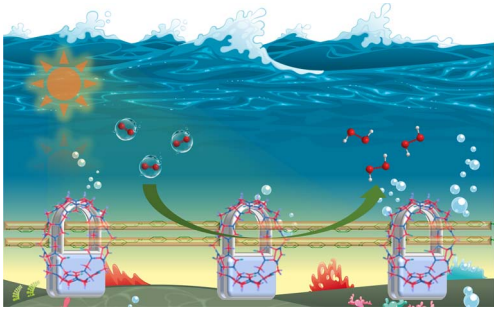
Cucurbit[8]uril as a supramolecular lock for designing a dual-chain conjugated polymer photocatalyst for enhanced H_2O_2 production

Jie Yin, Si-zhe Li, Hao Zhang, Yao Lu, Yan Zhao* and K. A. I. Zhang



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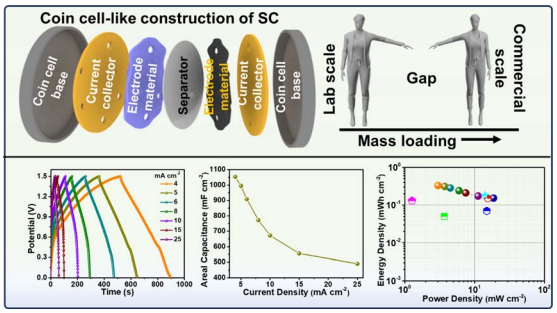
Polymer matrix-assisted commercial-level mass loading of porous cobalt manganese nitride towards high-performance binder-free electrodes for hybrid supercapacitors

Edugulla Girija Shankar, Ampasala Surya Kiran, Mandar Vasant Paranjape and Jae Su Yu*



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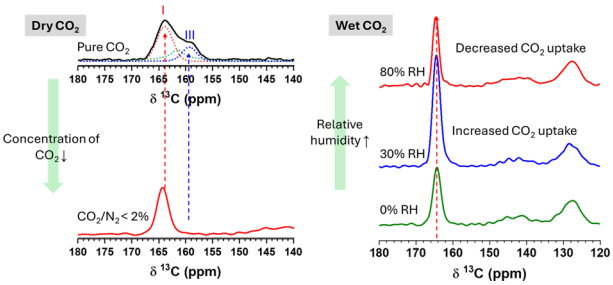
Discerning molecular-level CO_2 adsorption behavior in amine-modified sorbents within a controlled CO_2/H_2O environment towards direct air capture

Ah-Young Song, John Young, Jieyu Wang, Sophia N. Fricke, Katia Piscina, Raynald Giovine, Susana Garcia, Mijndert van der Spek and Jeffrey A. Reimer*



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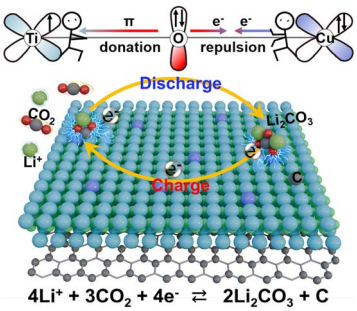
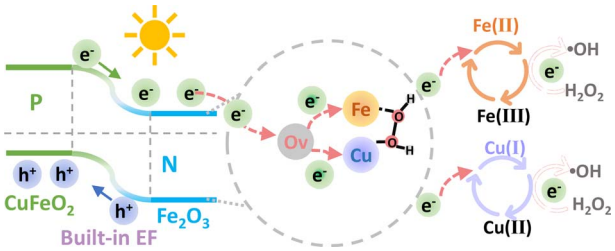


Boosted Li_2CO_3 reversible conversion utilizing Cu-doped TiB MBene/graphene for Li–CO_2 batteries

Tingting Luo, Qiong Peng,* Mengmeng Yang, Haojie Hu, Junfei Ding, Yanli Chen, Xiu Gong, Jingliang Yang, Yunpeng Qu, Zeyou Zhou, Xiaosi Qi* and Zhimei Sun*

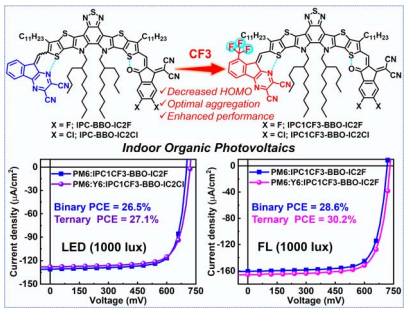
25896



Interlayer-release synthesis of Cu single atoms anchored on a heterogeneous photocatalyst for constructing Cu–O_v–Fe bimetallic active sites with ultrafast kinetics of activation of H_2O_2

Changdong Chen, Yan Shang, Shihui Shao, Wei Wang, Jiahao Zhu, Ying Gao, Lei Chen and Fangfang Wang*

25909



Trifluoromethyl-substituted asymmetric non-fullerene acceptors enable non-halogenated solvent-processed indoor organic photovoltaics with an efficiency of over 30%

Peddaboodi Gopikrishna, Muhammad Ahsan Saeed, SungHyun Hur, Gyeong Min Lee, Huijeong Choi, Jae Won Shim* and BongSoo Kim*

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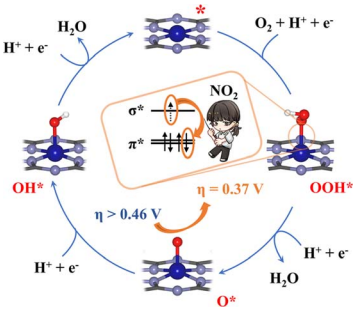

Boosting oxygen reduction reaction with metal phthalocyanines: altering central metals and substituents

Kunyu Li, Pai Wang, Jiarui Li, Yang Gao* and Yanning Zhang*

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PAPERS

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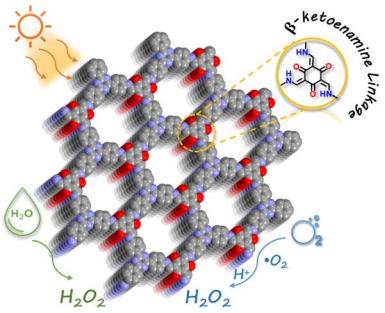
Integrating β-ketoenamine linkages into covalent organic frameworks toward efficient overall photocatalytic hydrogen peroxide production

Chang Shu, Peixuan Xie, Xiaoju Yang, Xuan Yang, Hui Gao, Bien Tan* and Xiaoyan Wang*



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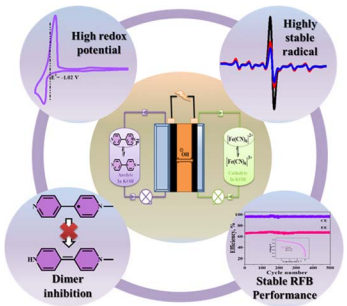
Mono-methyl viologen: a promising anolyte for alkaline aqueous redox flow batteries

Devendra Y. Nikumbe, R. Govindha Pandi, Anusuya Saha, Bhavana Bhatt, Surjit Bhai, Bishwajit Ganguly, Shanmugam Senthil Kumar and Rajaram K. Nagarale



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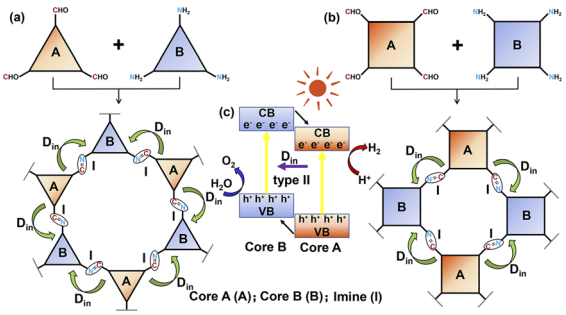
In-plane polarity boosts photocatalytic overall water splitting in two-dimensional covalent organic frameworks with polarized linkages

Yingcai Fan,* Zhihua Zhang, Xikui Ma* and Mingwen Zhao*



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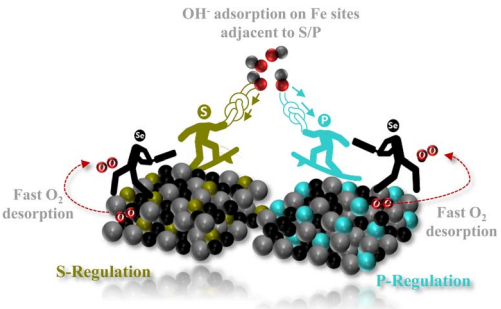
Boosting oxygen evolution kinetics *via* sulfur/phosphorus dynamic migration induced surface enrichment in an anion-regulated iron selenide

Bezawit Z. Desalegn, Reibelle Q. Raguindin, Gaojun Jiang, Hyung-Ho Park and Jeong Gil Seo*



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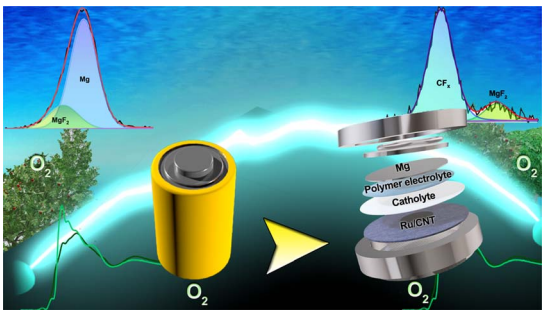
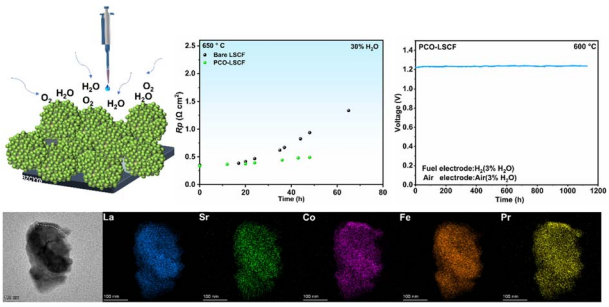


Polyethylene oxide-based solid-state polymer electrolyte hybridized with liquid catholyte for semi-solid-state rechargeable Mg–O_2 batteries

Ayan Sarkar, Shang-Yang Huang, Vasantan Rasupillai Dharmaraj, Behrouz Bazri, Kevin Iputera, Hsiu-Hui Su, Yi-An Chen, Han-Chen Chen, Yu-Ping Lin, Ren-Jei Chung,* Da-Hua Wei* and Ru-Shi Liu*

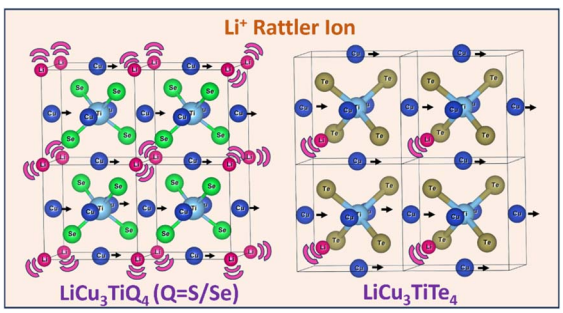
25979



Boosting steam tolerance and electrochemical performance of an $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$-based air electrode for protonic ceramic electrochemical cells

Lei Wu, Jiqiang Sun, Huiying Qi, Baofeng Tu, Chunyan Xiong, Fanglin Chen* and Peng Qiu*

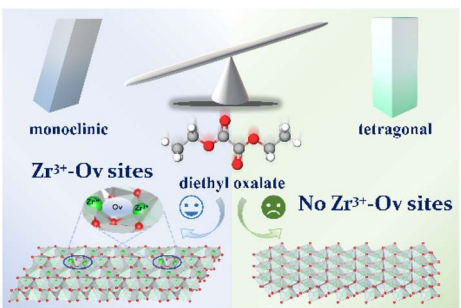
25988



Rattling induced bonding hierarchy in Li–Cu–Ti chalcotitanates for enhanced thermoelectric efficiency: a machine learning potential approach

Harpriya Minhas, Sandeep Das, Rahul Kumar Sharma and Biswarup Pathak*

26000



Crystalline phase effects of zirconia in Ag/ZrO_2 catalysts: oxygen vacancy-mediated new pathways to promote carbon–oxygen bond hydrogenation

Menghan Guo, Xiaofang Shang, Jiawei Li, Chenxi Yang, Jie Ding,* Qin Zhong* and Yixin Chen

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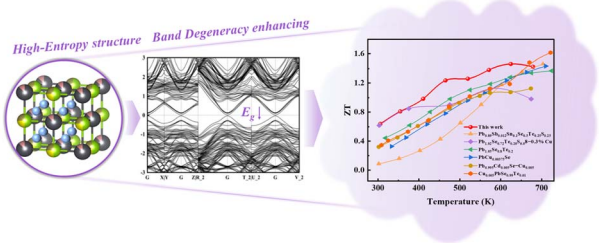
PAPERS

26013

Optimizing the thermoelectric performance of n-type PbSe through dynamic doping driven by entropy engineering

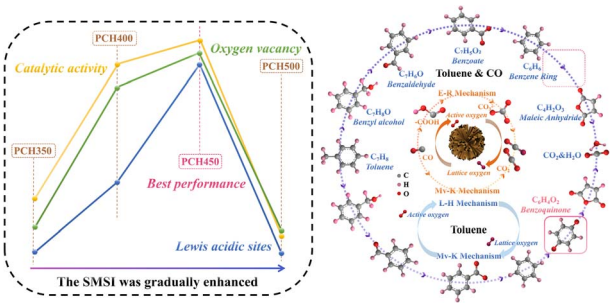
Shujie Wu, Changyuan Li, Feida Chen,* Kun Yang, Chengchao Hu, Haihua Huang, Wenjing Huang, Xueli Zuo and Xiaobin Tang*



26025

Boosting Lewis acidic sites *via* SMSI to enrich oxygen vacancies on Pt–CeO_2 catalysts: enhancing efficiency of CO promoted toluene catalysis

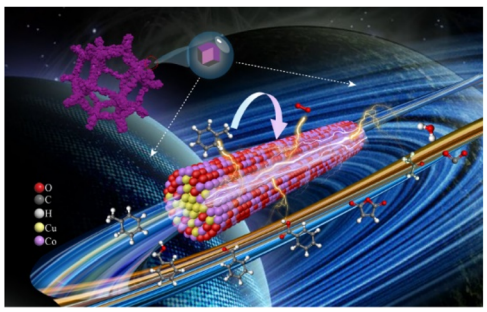
Xiaoying Zhou, Mingyuan Zhang,* Peiqi Mao, Jiaxuan Pang, Jiayi Wang, Liping Wang, Chentao Hou* and Daiqi Ye*



26038

Monolithic catalysts loaded with ZIF-derived Co_3O_4 on copper foam for the catalytic oxidation of toluene: the impact of synthetic methods

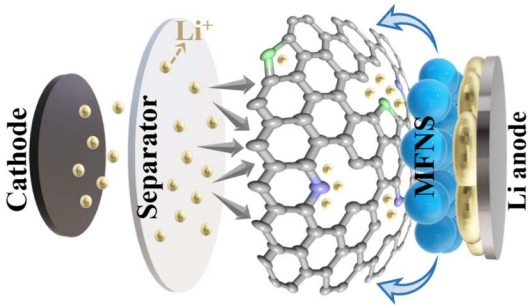
Wenju Liu, Zheng Zhang, Chen Zhu, Da Pan, Shaofeng Wang, Peng Jin, Fei Li, Yutong Shen and Dan Dang*



26056

A melamine–formaldehyde resin nanosphere interlayer as a "Li^+ redistributor" to stabilize Li metal anodes

Liang He, Qingjuan Ren,* Peng Zhang, Yujia Wang, Ruirui Hao, Kai Liu and Zhiqiang Shi*



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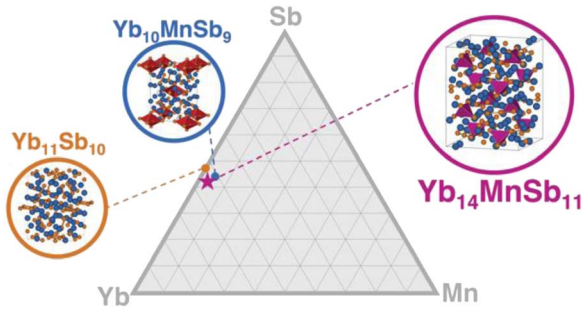
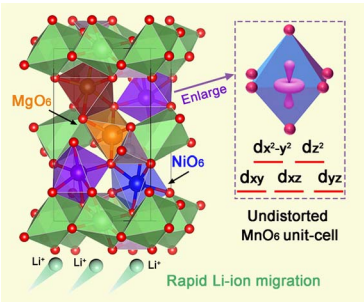
26064



The effects of $Yb_{11}Sb_{10}$ and $Yb_{10}MnSb_9$ secondary phases on the high performing thermoelectric material $Yb_{14}MnSb_{11}$

Leah Borgsmiller and G. Jeffrey Snyder*

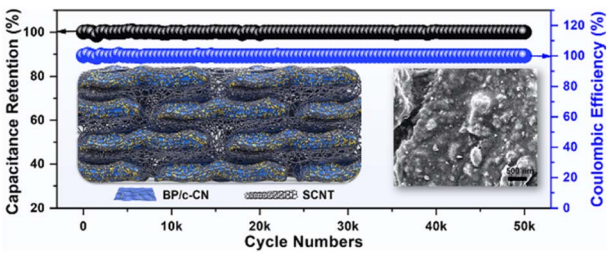
26076



Relaxing the Jahn–Teller distortion of $LiMn_{0.6}Fe_{0.4}PO_4$ cathodes *via* Mg/Ni dual-doping for high-rate and long-life Li-ion batteries

Haifeng Yu, Erdong Zhang, Jinxun Yu, Songmin Yu, Yaoguo Fang, Ling Chen,* Hao Jiang* and Chunzhong Li

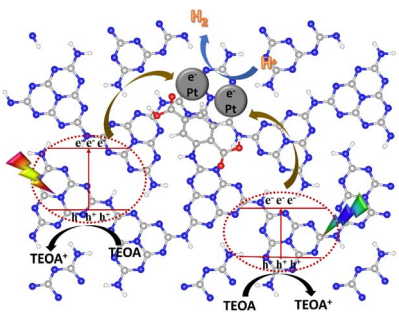
26083



Black phosphorus hybrid films enabled by a covalently chemical and spatial hierarchical-locking effect for flexible supercapacitors with 100% cycling stability

Xipeng Xin, Yifeng Xu, Min Zhou, Qingdong Liu, Jingyu Fan, Wei Chen, Jijin Xu, Jing Liu, Lian Gao, Kunpeng Zhao and Xuefeng Song*

26096



Simultaneously improving the delocalization of π electrons and directional transfer of charge carriers in carbon nitride for superior photocatalytic hydrogen evolution

Yujie Liang, Chi Cao, Lei Zeng,* Haonan Wang* and Yabin Jiang*

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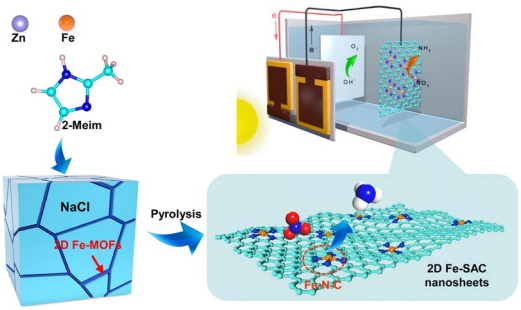
PAPERS

26103

Efficient solar-driven electrocatalytic nitrate-to-ammonia conversion by 2D ultrathin Fe single-atom catalysts

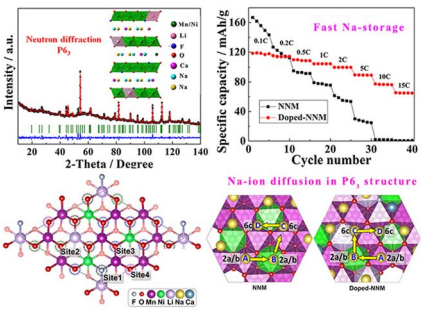
Ji Li,* Weiqi Zhong, Kai Wu, Eddy Petit, Luc Lajaunie, Kun Qi, Yang Zhang, Huali Wu, Jiefeng Liu, Jing Heng, Xuechuan Wang, Qingxin Han, Taotao Qiang and Damien Voiry*



26113

Promoting fast Na-storage and fabricating a stable layered cathode for sodium-ion batteries *via* site-selective substitution in triple crystallographic sites

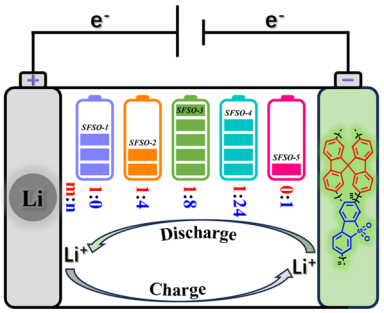
Zheng-Yao Li, Xiaobai Ma, Kai Sun,* Fanghua Ning,* Limei Sun, Gengfang Tian, Jianxiang Gao, Hongliang Wang and Dongfeng Chen*



26125

Influence of component molar ratios of conjugated polymers on the anode performance in lithium-ion batteries

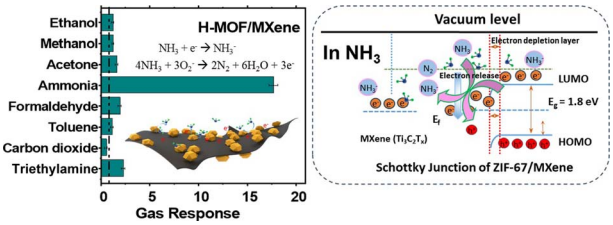
Detian Ma, Hui Xu, Yahui Zhang, Yuxuan Yang, Yunfei Bai,* Jincai Wu and Xiaobo Pan*



26132

Imparting hydrophobicity to a MOF on layered MXene for the selective, rapid, and ppb level humidity-independent detection of NH_3 at room temperature

Kugalur Shanmugam Ranjith, Sonam Sonwal, Ali Mohammadi, Ganji Seeta Rama Raju, Mi-Hwa Oh,* Yun Suk Huh* and Young-Kyu Han*



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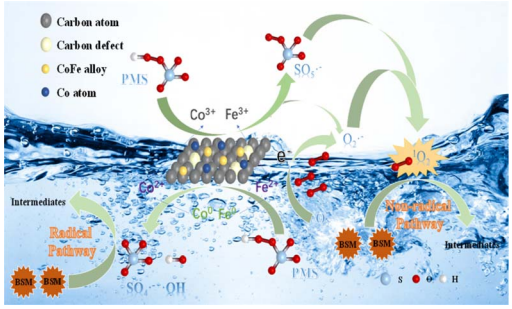
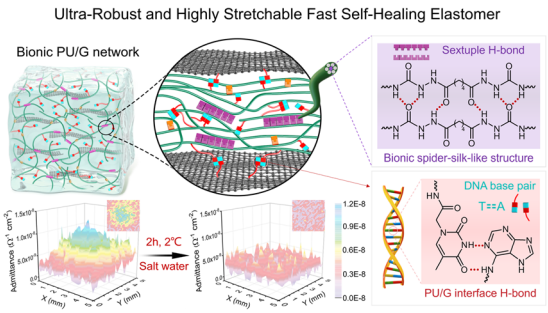
26147



Magnetic CoFe alloy–Co supported on mesoporous carbon as an efficient catalyst for the degradation of bensulfuron-methyl: insight into the effect of calcination temperature on carbon defects and singlet oxygen

Chao Yuan, Jialing Sheng, Shuke Guo, Xiaoyu Wang, Jiangyan Xu and Hongmei Jiang*

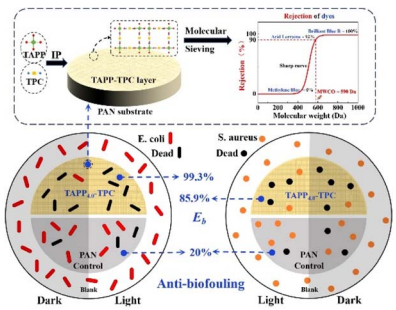
26158



Ultra-robust, highly stretchable and ambient temperature rapid self-healing polyurethane/graphene elastomers enabled by multi-type hydrogen bonds

Xiaobo Zhu, Yu Hao, Liang-Feng Huang, Haichao Zhao* and Liping Wang*

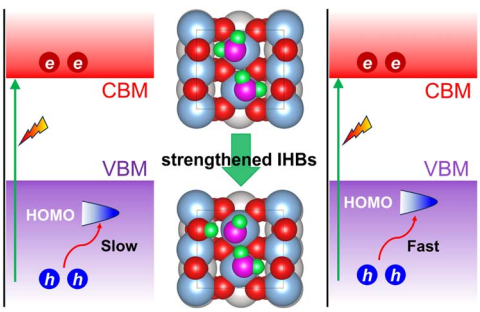
26170



A continuous porous porphyrinic polymer thin-film composite membrane for anti-biofouling and molecular sieving

Jia Xu,* Hansi Zhang, Xiaolong Ren, Shiyi Yao, Wenhua Fan, Ayman Nafady, Abdullah M. Al-Enizi and Shengqian Ma*

26178



Enhancement of hole capture and water dissociation on rutile TiO_2(110) by intermolecular hydrogen bonding: time-domain *ab initio* study

Yitong Zhang, Cheng Cheng, Yifan Wu, Oleg V. Prezhdo* and Run Long*

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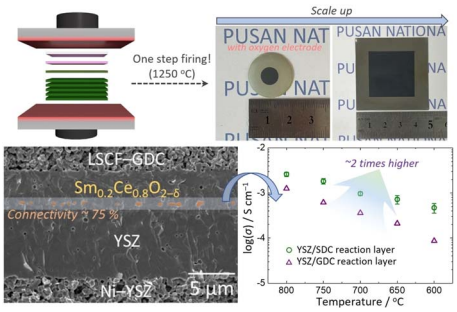
26188

Improved bi-layer electrolytes of solid oxide cells: the role of a $Sm_{0.2}Ce_{0.8}O_{2-\delta}$ diffusion barrier layer

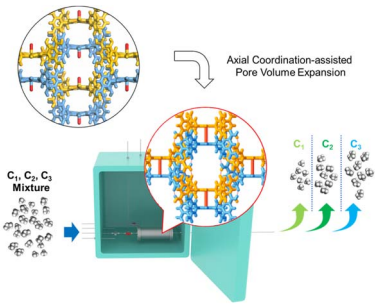
Su-Wan Kim, Hae-In Jeong, Dong-Yeon Kim and Beom-Kyeong Park*



26197

Axial coordination-assisted interwoven isomerism in 3D hydrogen-bonded organic frameworks for efficient natural gas purification

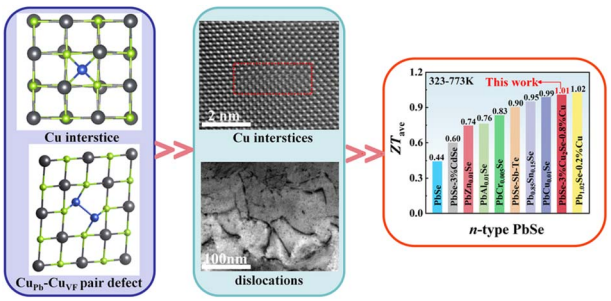
Hyunjun Park, Kwang Hyun Oh, Jae Hwa Lee, Younghun Kim, Jeong Heon Lee, Hoi Ri Moon,* Youn-Sang Bae* and Woo-Dong Jang*



26205

Complex lattice occupation of copper leading to enhanced thermoelectric performance in n-type PbSe

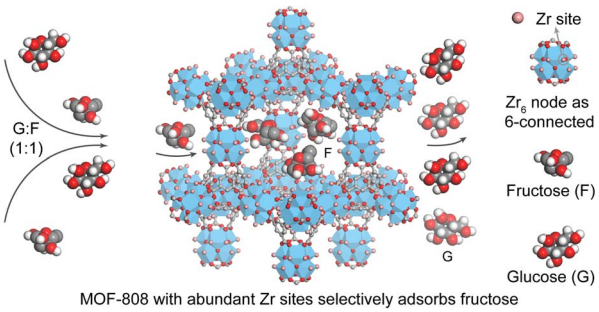
Yalin Shi, Mingkai He, Minchao Cui,* Weishuai Wang, Baopeng Ma, Fudong Zhang, Beiquan Jia, Xiaolian Chao, Zupei Yang* and Di Wu*



26214

High adsorption selectivity, capacity and rate of fructose using metal–organic frameworks with abundant zirconium open metal sites

Hai-Long He, Zhongqi Liu, Fengqing Liu, Jie Chen, Pu Wang, Xianfeng Yi, Anmin Zheng and Lei Wang*



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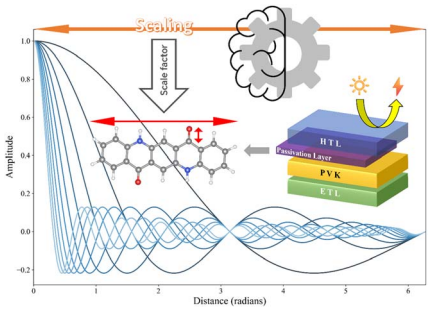
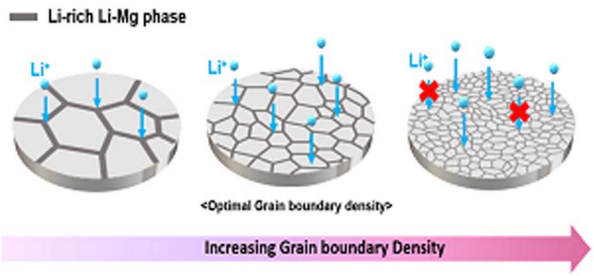


Explainable optimized 3D-MoRSE descriptors for the power conversion efficiency prediction of molecular passivated perovskite solar cells through machine learning

Xin Ye, Ningyi Cui, Wen Ou, Donghua Liu, Yufan Bao, Bin Ai* and Yecheng Zhou*

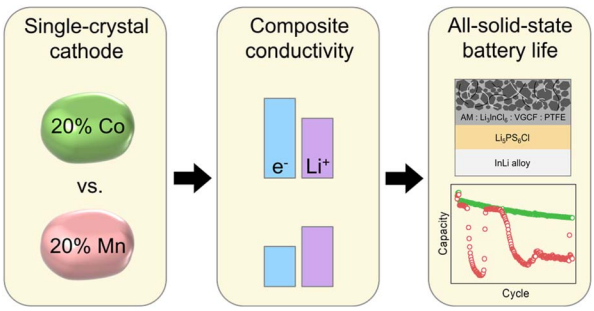
26234



Grain boundary optimization in Li–Mg alloy anodes *via* controlled cooling rates and cold rolling

Chae Yeon Yeom, Woo Seok Choi, Seung Ho Lee, Sin Hyong Joo, Jong Hoon Kim and Jong Hyeon Lee*

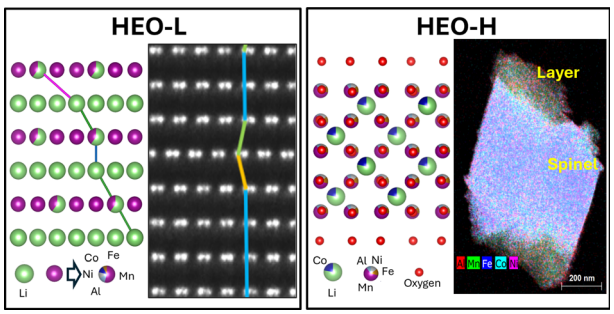
26244



Mixed ionic-electronic conductivity of high-nickel, single-crystal cathodes influencing the cycling stability of all-solid-state lithium-ion batteries

Steven Lee, Dongsoo Lee and Arumugam Manthiram*

26253



Manganese-rich high entropy oxides for lithium-ion batteries:materials design approaches to address voltage fade

Cynthia Huang, Jessica Luo, Zachary R. Mansley, Arun Kingan, Armando Rodriguez Campos, Zhongling Wang, Edelmy J. Marin Bernardez, Alexis Pace, Lu Ma, Steven N. Ehrlich, Lei Wang, David C. Bock, Esther S. Takeuchi, Amy C. Marschilok, Yimei Zhu, Shan Yan* and Kenneth J. Takeuchi*

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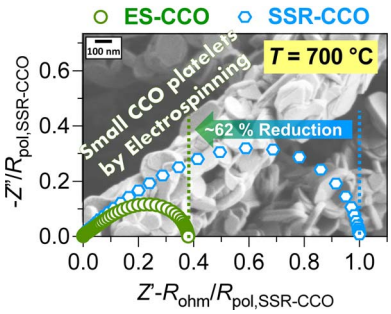
26266

Optimization of misfit calcium cobaltite oxygen electrodes for solid oxide fuel cells through electrospinning processing

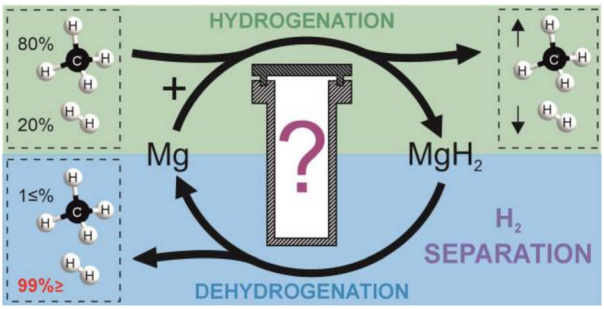
Allan J. M. Araújo,* Itzhak I. Maor, Laura I. V. Holz, Meirav Mann-Lahav, Vadim Beilin, Armin Feldhoff, Gideon S. Grader* and Francisco J. A. Loureiro*



26280

An insight into separating H_2 from natural gas/H_2 mixtures using Mg-based systems

Mateusz Balcerzak,* Robert Urbanczyk, Fabian Lange, Francis Anne Helm, Jan Ternieden and Michael Felderhoff



CORRECTION

26293

Correction: The effect of interface heterogeneity on zinc metal anode cyclability

J. T. Simon, V. Šedajová, D. Tripathy, H. E. Smith, S. M. Clarke,* C. P. Grey* and S. Menkin*