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Journal of Materials Chemistry A

Materials for energy and sustainability

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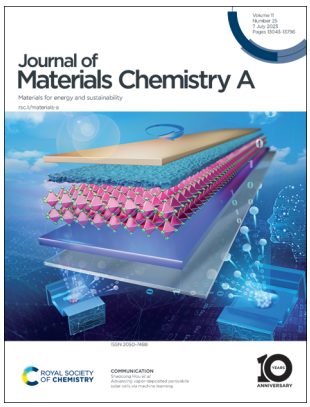

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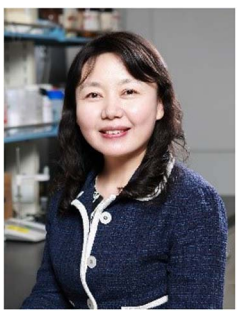
Inside cover
See Yunfeng Zhu, Rui Shi *et al.*, pp. 13255–13265. Image reproduced by permission of Yunfeng Zhu from *J. Mater. Chem. A*, 2023, **11**, 13255.

EDITORIAL

13063

Introduction to photofunctional materials and transformations

Li-Zhu Wu

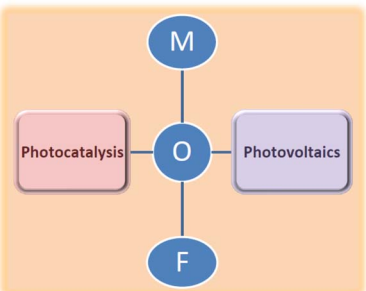


REVIEWS

13065

Photoelectroactive metal–organic frameworks

Cong Cong and Huaibo Ma*



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REVIEWS

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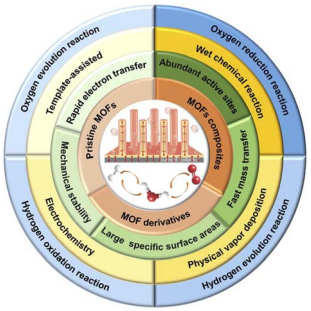
Self-supporting metal–organic framework-based hydrogen and oxygen electrocatalysts

Xinran Sun, Sibo Wang, Yidong Hou, Xue Feng Lu,* Jiujun Zhang and Xinchen Wang*



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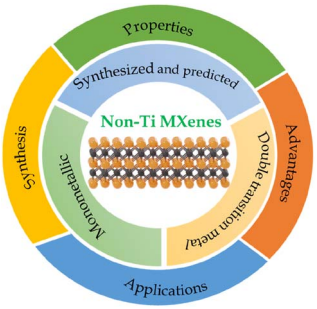
Recent advances in MXenes: beyond Ti-only systems

Sandhya Venkateshalu, Mohammed Shariq, Byeongyoon Kim, Monika Patel, Kajal Shakil Mahabari, Sang-Il Choi,* Nitin K. Chaudhari,* Andrews Nirmala Grace* and Kwangyeol Lee*



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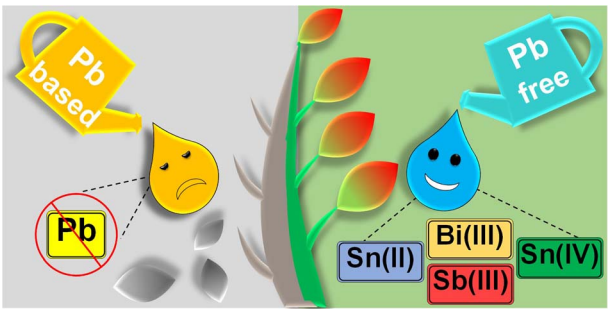
Design potential and future prospects of lead-free halide perovskites in photovoltaic devices

Mohammad Adil Afroz, Anupriya Singh, Ritesh Kant Gupta, Rabindranath Garai, Naveen Kumar Tailor, Yukta, Shivani Choudhary, Bhavna Sharma, Prerna Mahajan, Bhavya Padha, Sonali Verma, Sandeep Arya, Vinay Gupta, Seckin Akin, Daniel Prochowicz, Mohammad Mahdi Tavakoli, S. P. Singh, Parameswar K. Iyer, Pankaj Yadav, Hanlin Hu, Goutam De and Soumitra Satapathi*



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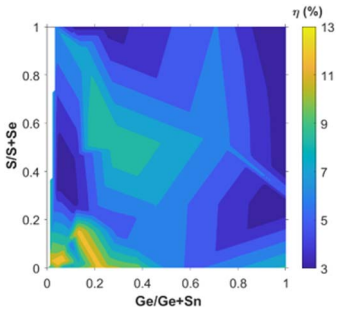
Ge-alloyed kesterite thin-film solar cells: previous investigations and current status – a comprehensive review

Romain Scaffidi,* Gizem Birant, Guy Brammertz, Jessica de Wild, Denis Flandre and Bart Vermang



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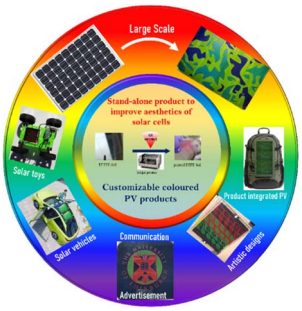

Visually attractive and efficient photovoltaics through luminescent downshifting

Neena Kurian Kalluvettukuzhy, Michal Robert Maciejczyk, Ian Underwood and Neil Robertson*

COMMUNICATIONS

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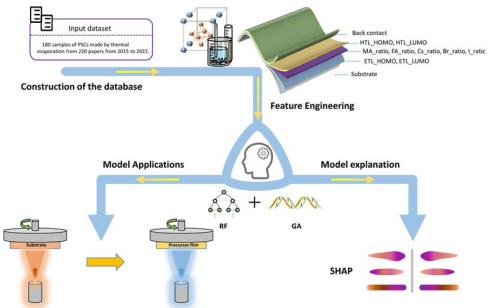

Advancing vapor-deposited perovskite solar cells *via* machine learning

Jiazheng Wang, Yuchen Qi, Haofeng Zheng, Ruilong Wang, Siyou Bai, Yanan Liu, Qi Liu, Jin Xiao, Dechun Zou and Shaocong Hou*

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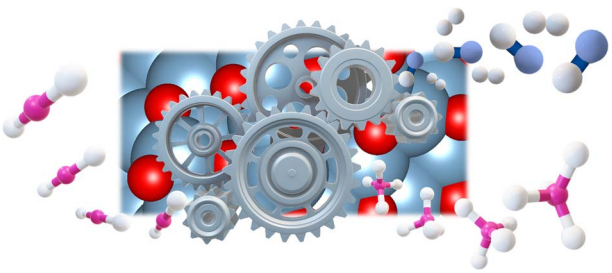

Unravelling the CO_2 capture and conversion mechanism of a NiRu–Na_2O switchable dual-function material in various CO_2 utilisation reactions

Loukia-Pantzechroula Merkouri, Juan Luis Martín-Espejo, Luis F. Bobadilla, José Antonio Odriozola, Anna Penkova, Tomas Ramirez Reina and Melis S. Duyar*

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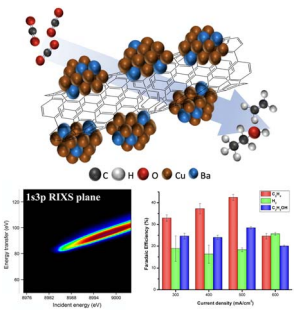

Copper–barium-decorated carbon-nanotube composite for electrocatalytic CO_2 reduction to C2 products

Feng-Yi Wu, Hsin-Jung Tsai, Tsung-Ju Lee, Zih-Yi Lin, Kang-Shun Peng, Pei-Hsuan Chen, Nozomu Hiraoka, Yen-Fa Liao, Chih-Wei Hu, Shao-Hui Hsu, Ying-Rui Lu* and Sung-Fu Hung*

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COMMUNICATIONS

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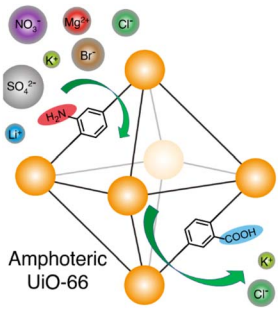
Amphoteric metal–organic framework subnanochannels with pH-tuneable cation and anion sieving properties

Jue Hou,* Huacheng Zhang, Huanting Wang, Aaron W. Thornton and Kristina Konstas*



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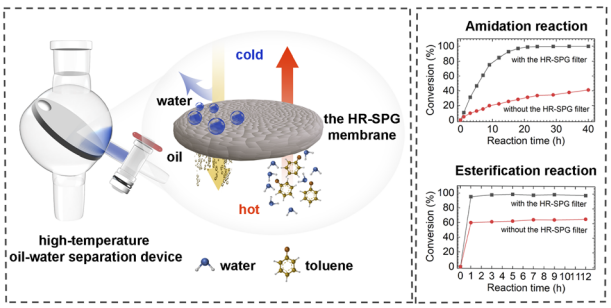
High temperature oil–water separation based on superwettable membranes for removing water from condensation reactions

Wenting Zhou, Fan Min, Jing Shi, Deqi Wang, Haikang Huang, Hengchang Liu and Zonglin Chu*



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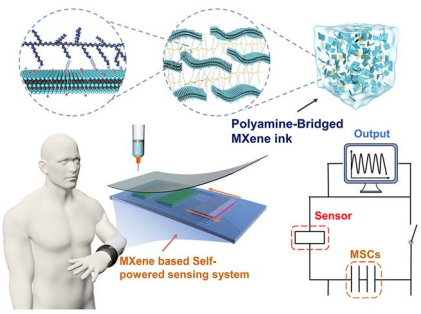
Monolithically integrated flexible sensing systems with multi-dimensional printable MXene electrodes

Shuiren Liu,* Qi Meng, Yadong Gao, Juzhong Zhang, Jiarong Li, Youwei Yang, Xiaomeng Zhang, Hongpeng Li and Xuying Liu*



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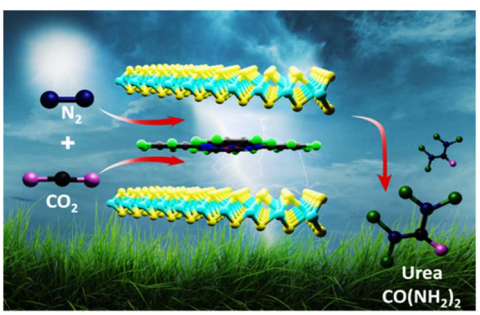
Dual metal site-mediated efficient C–N coupling toward electrochemical urea synthesis

Sourav Paul, Sougata Sarkar, Ashadul Adalder, Amitava Banerjee and Uttam Kumar Ghorai*



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PAPERS

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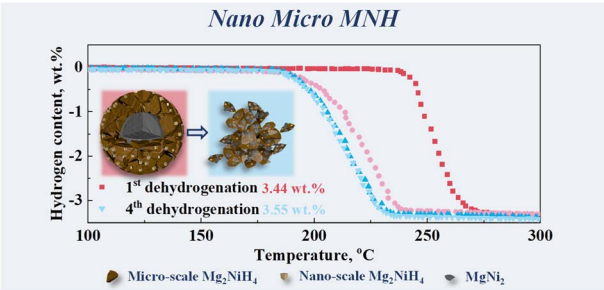

Structural inhomogeneity: a potential strategy to improve the hydrogen storage performance of metal hydrides

Yingyan Zhao, Yunfeng Zhu,* Rui Shi,* Zhen Jia, Jiguang Zhang, Yana Liu, Honghui Cheng, Qinke Tang, Zhixin Ba, Xiaohui Hu and Liquan Li

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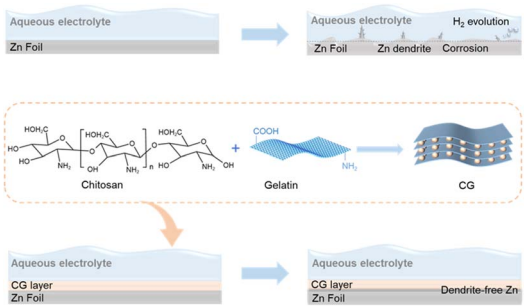

High performance Zn anodes enabled by a multifunctional biopolymeric protective layer for a dendrite-free aqueous zinc-based battery

Lingzhi Kang, Jiale Zheng, Huadong Yuan, Jianmin Luo, Yao Wang, Yujing Liu, Jianwei Nai and Xinyong Tao*

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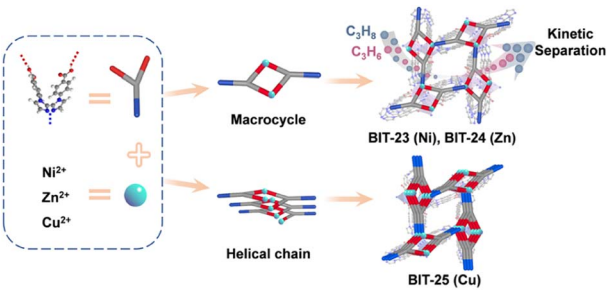

Rational design of metal–organic frameworks featuring macrocycle and helical chain motifs for propylene/propane separation

Xinyu Yu, Xin Huang, Mengchu Feng, Yuanyuan Zhang* and Bo Wang*

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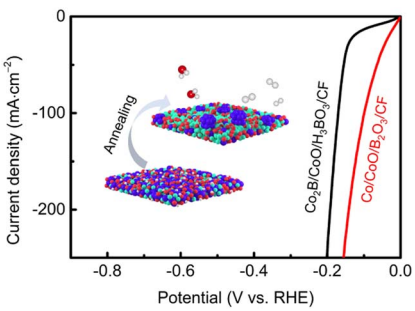

Boride-mediated synthesis of a highly active cobalt-based electrocatalyst for alkaline hydrogen evolution reaction

Yanmei Ren, Jiajun Wang, Weizhen Wang, He Wen, Muhua Chen, Yuping Qiu, Guangyao Li, Zhiqing Yang and Ping Wang*

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PAPERS

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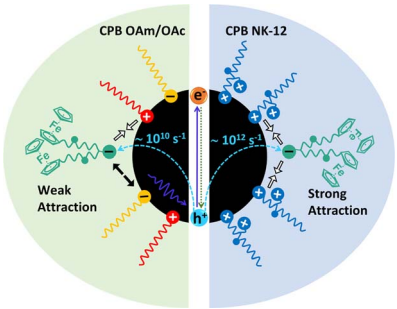
Synergistic binding between an engineered interface and functionalized ferrocene offers remarkable charge extraction efficiency in lead halide perovskites

Monika Ahlawat, Santosh Kumari and Vishal Govind Rao*



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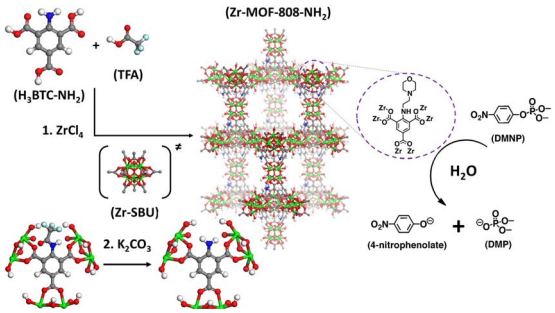
Enhancement of catalytic hydrolysis activity for organophosphates by the metal–organic framework MOF-808-NH_2 *via* post-synthetic modification

Sergio J. Garibay, Trenton M. Tovar, Ivan O. Iordanov, Gregory W. Peterson and Jared B. DeCoste*



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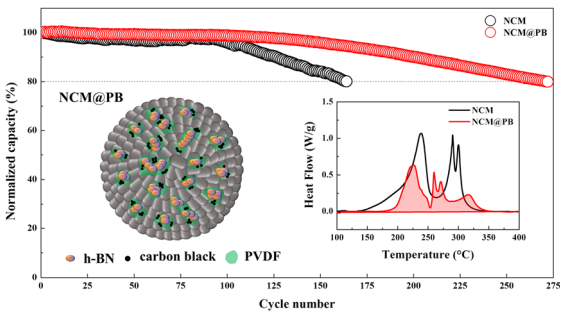
A boron-nitride based dispersive composite coating on nickel-rich layered cathodes for enhanced cycle stability and safety

Hsi Chen, Yan-Cheng Chen, Hao-Wen Liu, Shu-Jui Chang, Cheng-Hung Liao, Senthil-Kumar Parthasarathi, Satish Bolloju, Yu-Ting Weng, Jyh-Fu Lee, Jin-Ming Chen, Hwo-Shuenn Sheu, Chih-Wen Pao and Nae-Lih Wu*



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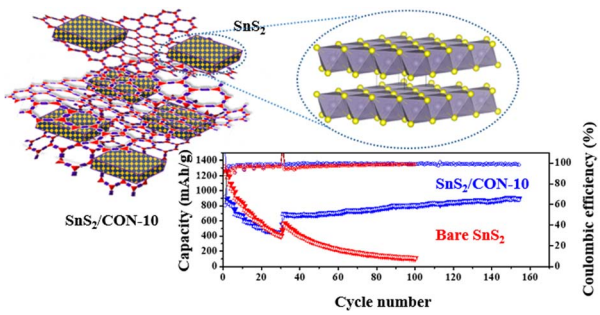
Long-term cycling stability of a SnS_2-based covalent organic nanosheet anode for lithium-ion batteries

Jeong-Hun Jang, Minseop Lee, Soohyeon Park, Jae-Min Oh,* Jin Kuen Park* and Seung-Min Paek*



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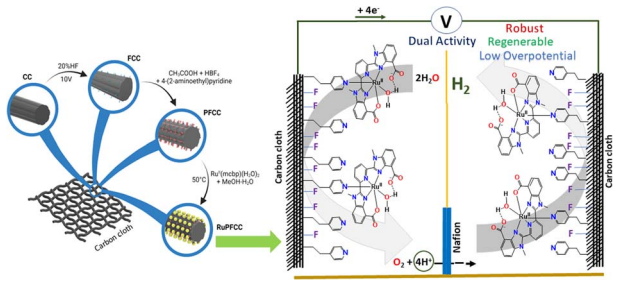
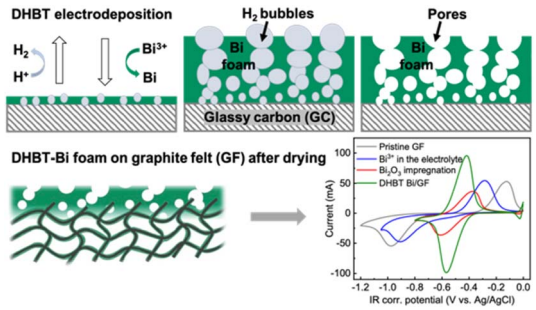


Bifunctional and regenerable molecular electrode for water electrolysis at neutral pH

Biswanath Das,* Esteban A. Toledo-Carrillo, Guoqi Li, Jonas Ståhle, Thomas Thersleff, Jianhong Chen, Lin Li, Fei Ye, Adam Slabon, Mats Göthelid, Tsu-Chien Weng, Jodie A. Yuwono, Priyank V. Kumar, Oscar Verho,* Markus D. Kärkäs, Joydeep Dutta and Björn Åkermark*

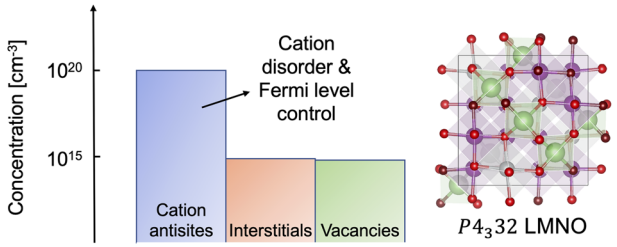
13341



Dynamic hydrogen bubble template electrodeposited Bi on graphite felt and the effect of its post-processing in vanadium redox flow batteries

Ming Cheng, Tintula Kottakkat* and Christina Roth

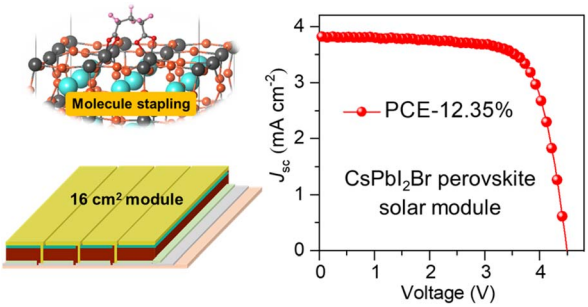
13353



Cation disorder dominates the defect chemistry of high-voltage $LiMn_{1.5}Ni_{0.5}O_4$ (LMNO) spinel cathodes

Jiayi Cen, Bonan Zhu, Seán R. Kavanagh, Alexander G. Squires and David O. Scanlon*

13371



Molecule stapling-assisted fabrication of high-quality $CsPbI_2Br$ films for efficient and stable photovoltaic modules

Ruihao Chen,* Jieru Du, Xuan Zheng, Yuyao Yang, Li Yuan, Yang Yang, Feiming Li and Hongqiang Wang*

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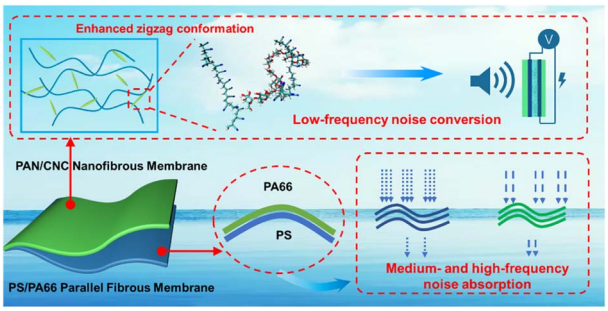
13378

High-efficiency absorption and acoustoelectric conversion in heterogeneous nanofibers: a two-pronged approach to full-frequency de-noising

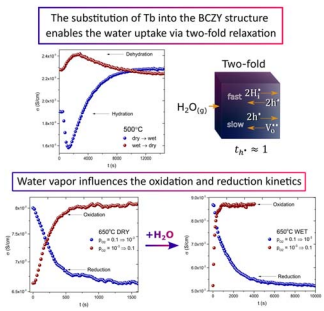
Ziyao Fan, Shuanglin Wu, Kaiyang Fang, Feng Tang, Leibing Zhang and Fenglin Huang*



13389

Water uptake kinetics and electrical transport in $BaCe_{0.6}Zr_{0.2}Y_{0.1}M_{0.1}O_{3-\delta}$ (M = Tb, Pr, Fe) protonic conductors

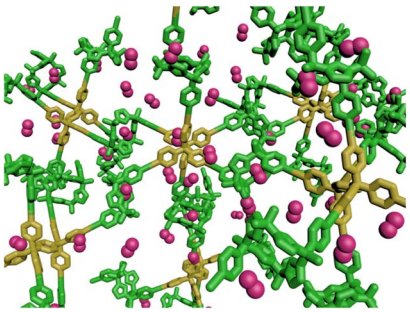
Jagoda Budnik,* Aleksandra Mielewczyk-Gryń, Maria Gazda and Tadeusz Miruszewski*



13399

Macrocycle polymeric networks based on a chair-like calix[4]pyrrole for the rapid and efficient adsorption of iodine from water

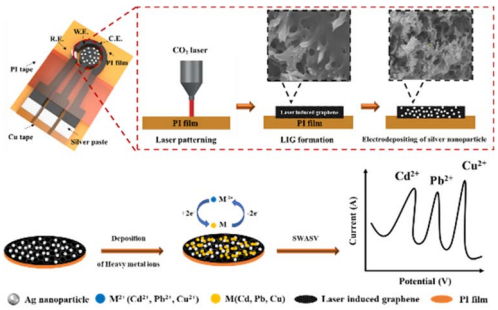
Zhiye Zheng, Qiuyuan Lin, Linhuang Xie, Xiaolong Chen, Huan Zhou, Kunhua Lin, Dengsong Zhang, Xiaodong Chi, Jonathan L. Sessler* and Hongyu Wang*



13409

Laser-induced graphene incorporated with silver nanoparticles applied for heavy metal multi-detection

Seongeun Jeong, Sungwook Yang, Yi Jae Lee and Soo Hyun Lee*



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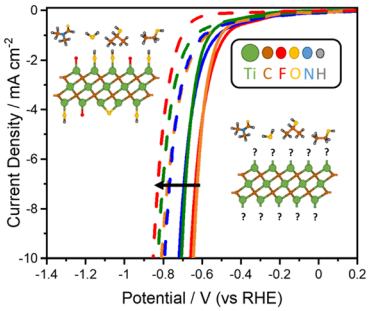
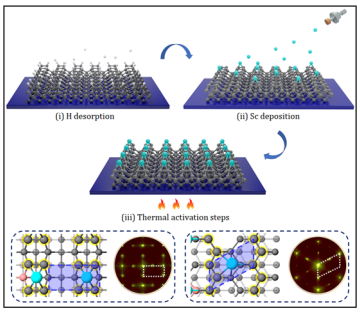
13419



Solvents dramatically influence the atomic composition and catalytic properties of $Ti_3C_2T_x$ MXenes

Katarina A. Novčić, Christian Iffelsberger, Mario Palacios-Corella and Martin Pumera*

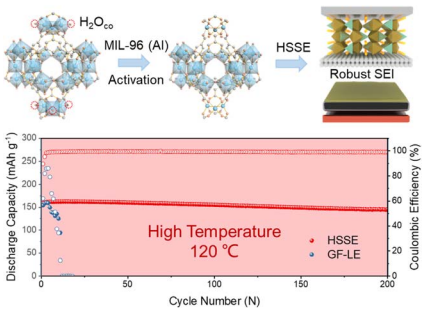
13432



Experimental evidence for large negative electron affinity from scandium-terminated diamond

Ramiz Zulkharnay* and Paul W. May

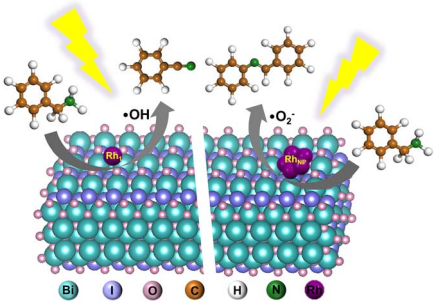
13446



A hybrid solid-state electrolyte endows a Li metal battery with excellent cycling life at 120 °C

Wen-Xue Liu, Xue-Chun Huang, Yan Meng,* Dan Xiao* and Yong Guo*

13459



Tuning the selectivity of benzylamine photo-oxidation with different rhodium modes anchored on $BiOIO_3$

Jiaping Liu, Yan Wu, Qingqing Chen, Rui Yu, Keqing Shi, Tao Jing, Zhujie Li,* Zaizhu Lou* and Gang Wang*

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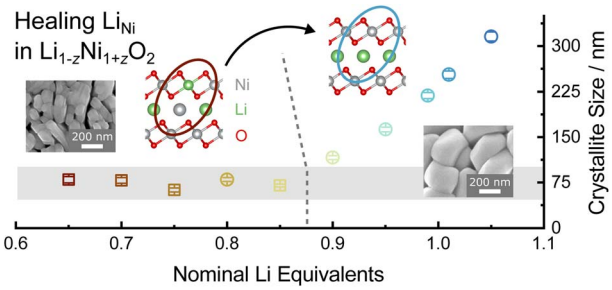
13468

Stoichiometry matters: correlation between antisite defects, microstructure and magnetic behavior in the cathode material $Li_{1-z}Ni_{1+z}O_2$

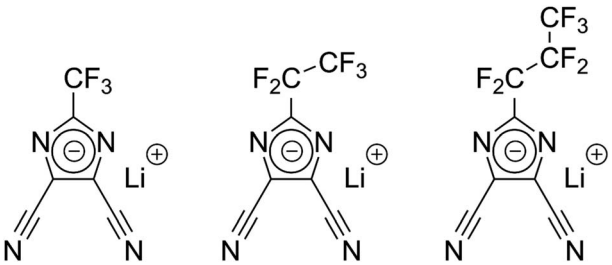
Damian Goonetilleke, Björn Schwarz, Hang Li, Francois Fauth, Emmanuelle Suard, Stefan Mangold, Sylvio Indris, Torsten Brezesinski, Matteo Bianchini and Daniel Weber*



13483

Ionic conductivity, viscosity, and self-diffusion coefficients of novel imidazole salts for lithium-ion battery electrolytes

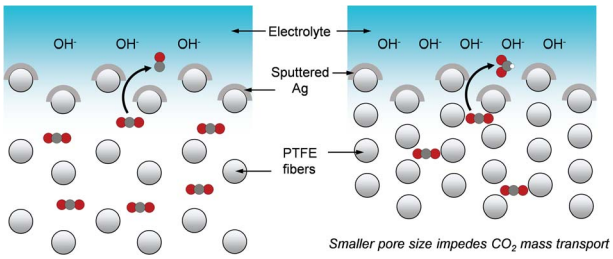
Anna Szczęsna-Chrzan, Monika Vogler, Peng Yan, Grażyna Zofia Żukowska, Christian Wölke, Agnieszka Ostrowska, Sara Szymańska, Marek Marcinek, Martin Winter, Isidora Cekic-Laskovic,* Władysław Wieczorek* and Helge S. Stein*



13493

Local microenvironment tuning induces switching between electrochemical CO_2 reduction pathways

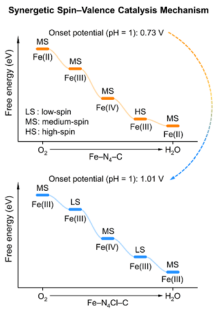
Surani Bin Dolmanan, Annette Böhme, Ziting Fan, Alex J. King, Aidan Q. Fenwick, Albertus Denny Handoko, Wan Ru Leow, Adam Z. Weber, Xinbin Ma, Edwin Khoo, Harry A. Atwater* and Yanwei Lum*



13502

Synergistic spin–valence catalysis mechanism in oxygen reduction reactions on Fe–N–C single-atom catalysts

Daoxiong Wu, Zhiwen Zhuo, Yiming Song, Peng Rao, Junming Luo, Jing Li, Peilin Deng,* Jinlin Yang, Xiaojun Wu and Xinlong Tian*



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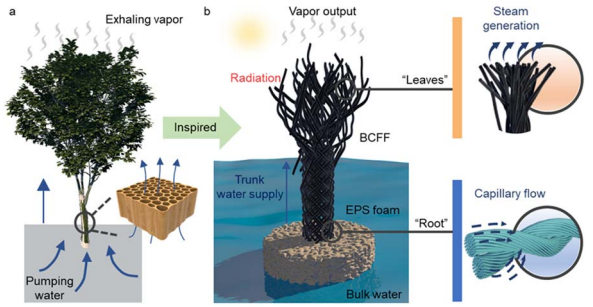
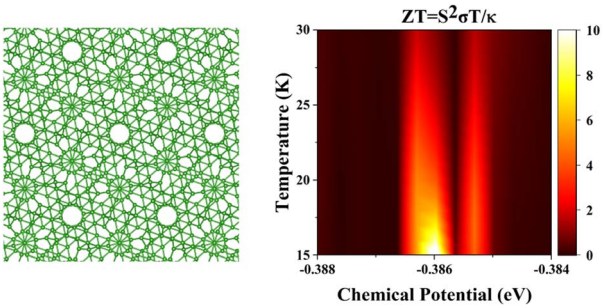
13510



Tree-inspired braiding fibrous frameworks enabling high-efficiency and salt-rejecting solar evaporation

Duo Xu, Can Ge, Ze Chen, Yingcun Liu, Tao Chen, Chong Gao, Keshuai Liu, Weilin Xu, Qian Zhang* and Jian Fang*

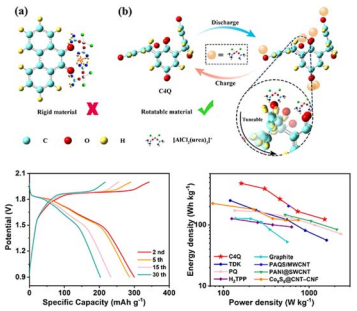
13519



Challenging breaking thermoelectric performance limits by twistronics

Jizhe Song and Mengtao Sun*

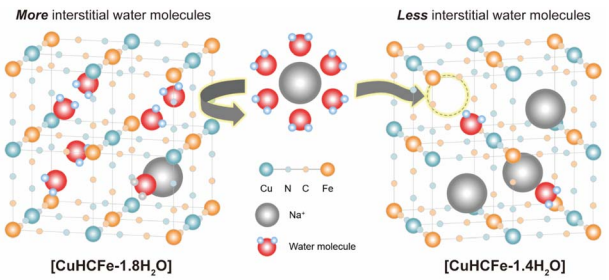
13527



A rotatable cathode with tunable steric hindrance for high-performance aluminum organic batteries

Mingshan Han, Qinqin Zhou, Meng Zhang, Jinshu Wang,* Fangyan Cui, Yunfei Yang, Jingwen Su, Weiwei Huang* and Yuxiang Hu*

13535



Investigating the role of interstitial water molecules in copper hexacyanoferrate for sodium-ion battery cathodes

Donghyeon Kim, Ahreum Choi,* Changhyun Park, Min-Ho Kim and Hyun-Wook Lee*

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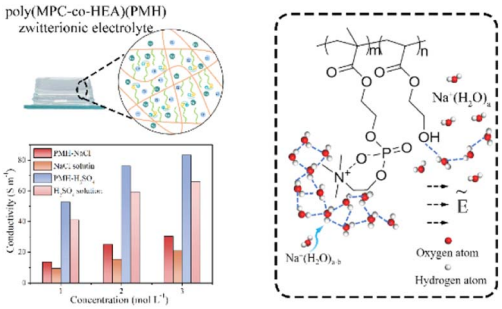
13543

A zwitterionic hydrogel with a surprising function of increasing the ionic conductivity of alkali metal chloride or sulfuric acid water-soluble electrolyte

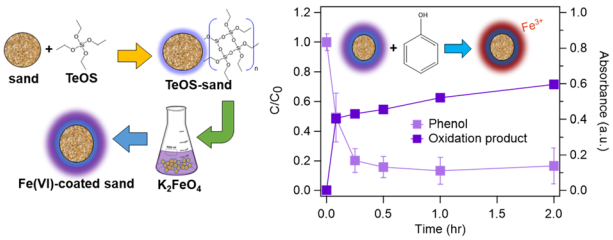
Danchen Fu, Yanfen Lu, Zhiyuan Peng and Wenbin Zhong*



13552

Synthesis of ferrate (Fe(VI))-coated sand for stabilized reactivity and enhanced treatment of phenol

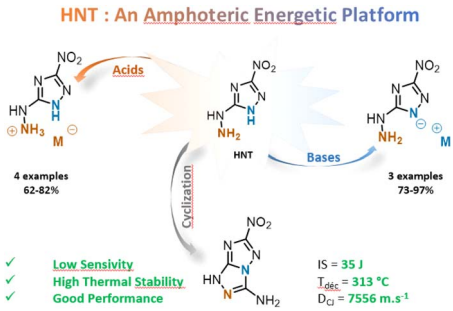
Fanny E. K. Okaikue-Woodi and Jessica R. Ray*



13564

Synthesis and reactivity of 5-hydrazino-3-nitro-1,2,4-triazole (HNT): an amphoteric energetic platform

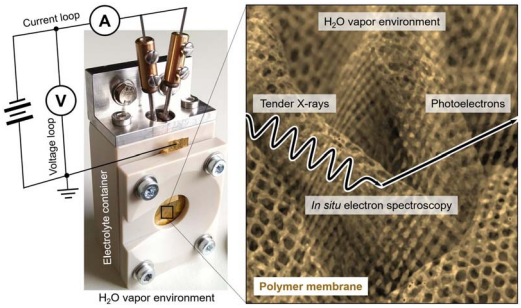
Loïc Habert, Matthieu Daniel, Pascal Palmas and Eric Pasquinet*



13570

***In situ* investigation of ion exchange membranes reveals that ion transfer in hybrid liquid/gas electrolyzers is mediated by diffusion, not electromigration**

Maryline Ralaiarisoa, Senapati Sri Krishnamurti, Wenqing Gu, Claudio Ampelli, Roel van de Krol, Fatwa Firdaus Abdi* and Marco Favaro*



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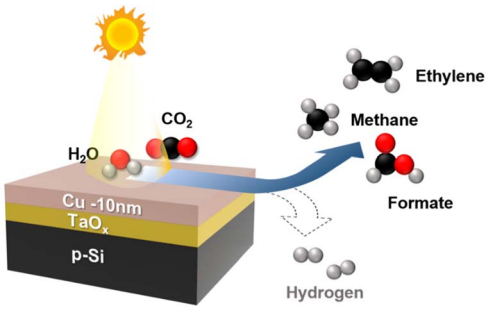
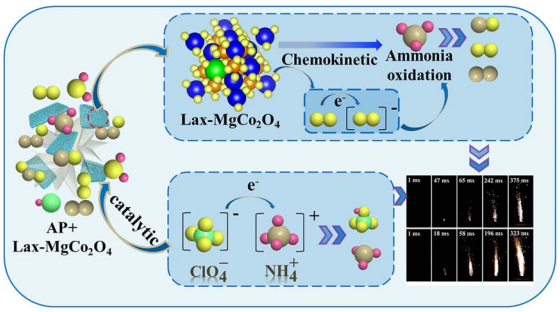


TaO_x electron transport layers for CO_2 reduction Si photocathodes

Rajiv Ramanujam Prabhakar, Raphaël Lemerle, Magda Barecka, Minki Kim, Sehun Seo, Elif Nur Dayi, Irene Dei Tos and Joel W. Ager*

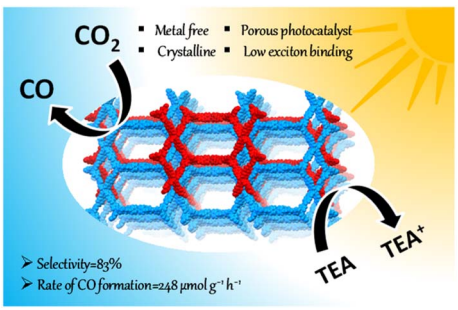
13600



A strategy for modulating the catalytic active center of AP thermal decomposition and its application: La-doped $MgCo_2O_4$

Guofei Zhang, Xin Yu, Zhenlong Wang, Sirong Li, Zhengyi Zhao, Yunjiong Zhu, Yude Wang* and Xuechun Xiao*

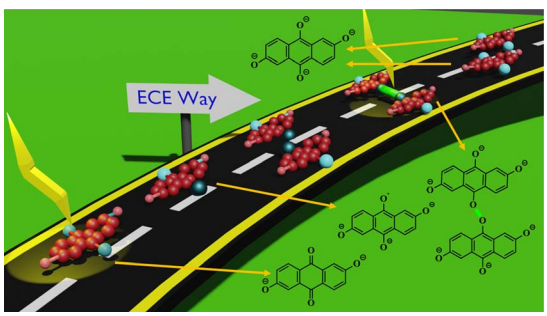
13615



Metal-free 3D donor–acceptor COF with low exciton binding for solar fuel production based on CO_2 reduction

Anupam Dey, Faruk Ahamed Rahimi, Soumitra Barman, Arpan Hazra and Tapas Kumar Maji*

13623



Use of voltage for recomposing degraded redox active molecules for flow battery applications

Abhilipsa Sahoo and Kothandaraman Ramanujam*

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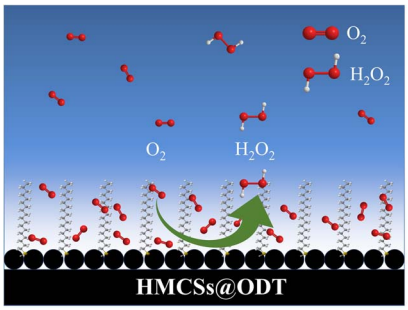
13633

Interface engineering of superhydrophobic octadecanethiol-functionalized hollow mesoporous carbon spheres for alkaline oxygen reduction to hydrogen peroxide

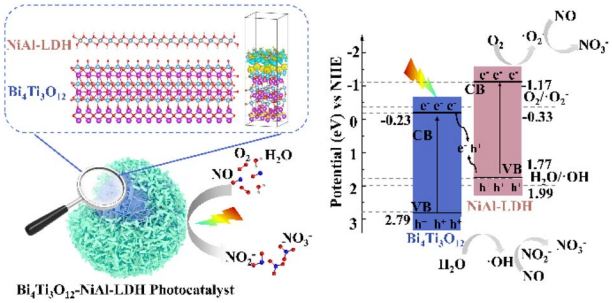
Hongjing Wang, Shaojian Jiang, Hongjie Yu,* Kai Deng, Ziqiang Wang, Xiaonian Li, You Xu and Liang Wang*



13640

Efficient photocatalytic NO oxidation over novel NiAl layered double hydroxide/$Bi_4Ti_3O_{12}$ Z-scheme heterojunctions with boosted charge separation and O_2 activation

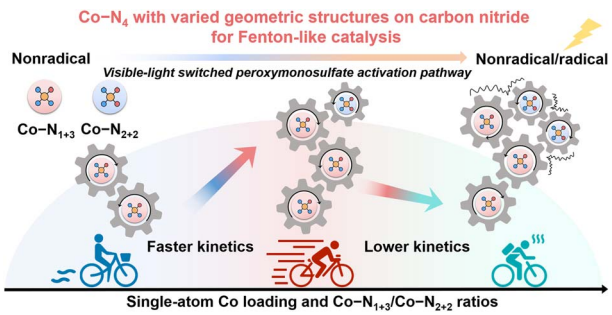
Guojun Li, Yue Deng, Ting Li, Zheng Lian, Qiuqiu Lyu, Zhinian Liu, Shule Zhang* and Qin Zhong*



13653

The structure-dependent mechanism of single-atom cobalt on macroporous carbon nitride in (photo-) Fenton-like reactions

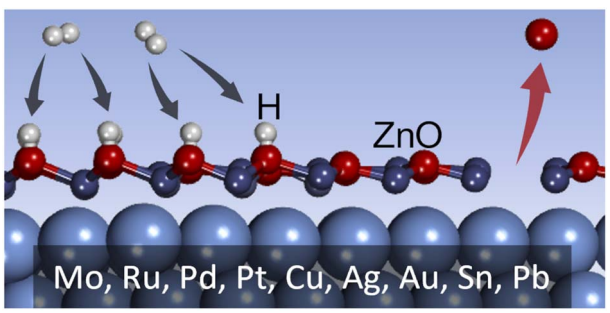
Jingkai Lin, Lin Jiang, Wenjie Tian, Yangyang Yang, Xiaoguang Duan, Yan Jiao,* Huayang Zhang* and Shaobin Wang*



13665

Tunable properties and composition of ZnO films supported on metal surfaces

Yizhen Song, Paulo C. D. Mendes and Sergey M. Kozlov*



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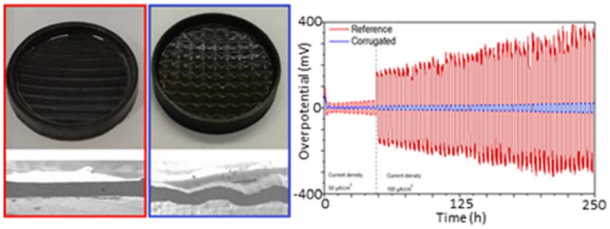
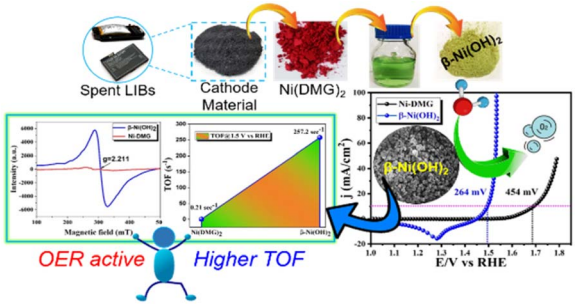


3D printing of self-supported solid electrolytes made of glass-derived $Li_{1.5}Al_{0.5}Ge_{1.5}P_3O_{12}$ for all-solid-state lithium-metal batteries

A. G. Sabato,* M. Nuñez Eroles, S. Anelli, C. D. Sierra, J. C. Gonzalez-Rosillo, M. Torrell, A. Pesce, G. Accardo, M. Casas-Cabanas, P. López-Aranguren, A. Morata and A. Tarancón*

13687



Waste is the best: end-of-life lithium ion battery-derived ultra-active Ni^{3+}-enriched β-$Ni(OH)_2$ for the electrocatalytic oxygen evolution reaction

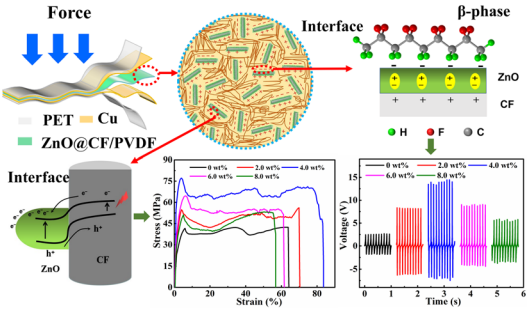
Hiren Jungi, Arun Karmakar, Subrata Kundu* and Joyee Mitra*

13697

Novel high-entropy layered double hydroxide microspheres as an effective and durable electrocatalyst for oxygen evolution

Shun Li, Likai Tong, Zhijian Peng,* Bo Zhang and Xiuli Fu*

13708



High-performance piezoelectric nanogenerators based on hierarchical ZnO@CF/PVDF composite film for self-powered meteorological sensor

Yinhui Li,* Jiaojiao Sun, Pengwei Li, Xuran Li, Jianqiang Tan, Hulin Zhang, Tingyu Li, Jianguo Liang, Yunlei Zhou, Zhenyin Hai* and Jin Zhang*

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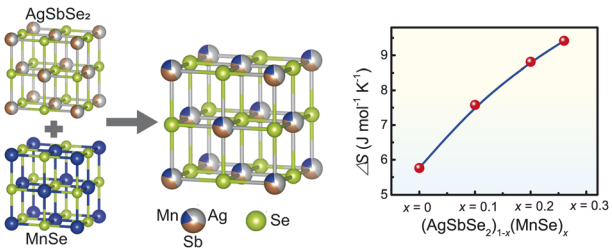
Enhancing the solubility of Mn in $AgSbSe_2$ for high thermoelectric performance through entropy engineering

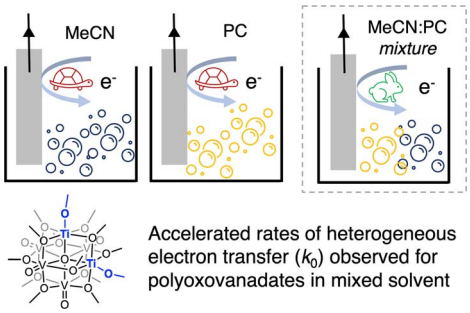
Zheng Ma, Yubo Luo,* Wang Li, Yingchao Wei, Chengjun Li, Abubakar Yakubu Haruna, Zhihong Zhang, Xin Li, Qinghui Jiang and Junyou Yang*



13729

Solvent mixtures for improved electron transfer kinetics of titanium-doped polyoxovanadate-alkoxide clusters

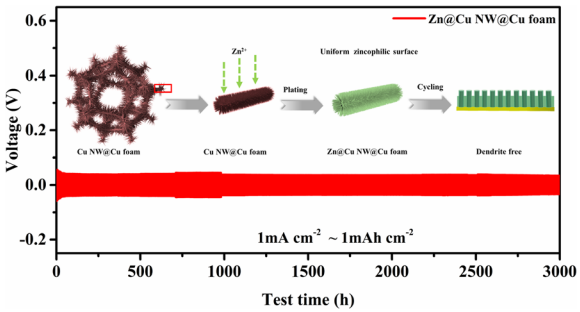
Mamta Dagar, Molly Corr, Timothy R. Cook, James R. McKone* and Ellen M. Matson*



13742

Constructing a well-wettable interface on a three-dimensional copper foam host with reinforced copper nanowires to stabilize zinc metal anodes

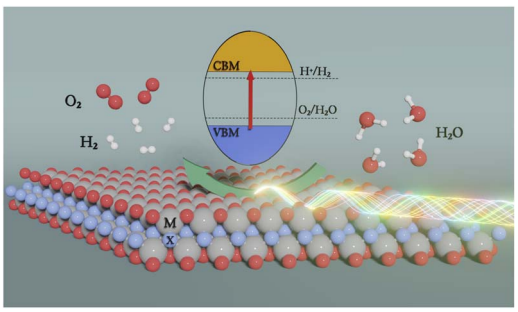
Yixing Fang, Kun Han, Zhen Wang, Jie Shi, Ping Li* and Xuanhui Qu*



13754

Bandgap engineering of MXene compounds for water splitting

Diego Ontiveros, Francesc Viñes and Carmen Sousa*



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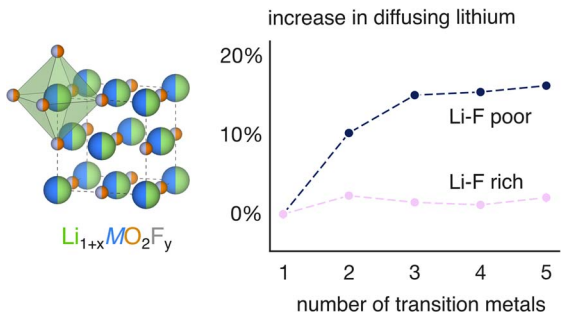
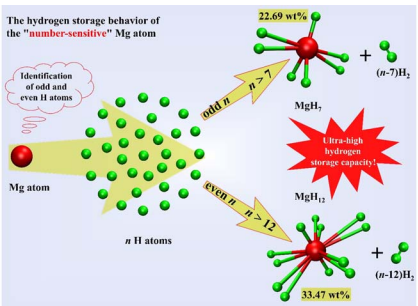
13765



Understanding the limits to short-range order suppression in many-component disordered rock salt lithium-ion cathode materials

Alexander G. Squires* and David O. Scanlon*

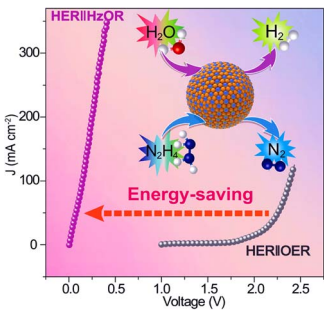
13774



Study of the hydrogen absorption behaviour of a "number-sensitive" Mg atom: ultra-high hydrogen storage in MgH_n ($n = 1$–20) clusters

Ben-Chao Zhu, Guang-Hui Liu, Ping-Ji Deng, Chun-Jing Liu, Yan-Hua Liao,* Lu Zeng* and Jun Zhao*

13783



Regulating Ru active sites by Pd alloying to significantly enhance hydrazine oxidation for energy-saving hydrogen production

Simeng Zhao, Yankai Zhang, Haibo Li, Suyuan Zeng, Rui Li, Qingxia Yao, Hongyan Chen, Yao Zheng* and Konggang Qu*

CORRECTION

13793

Correction: Crystal growth of two-dimensional organic–inorganic hybrid perovskites and their application in photovoltaics

Yuling Zhang, Ruyue Wang and Zhan'ao Tan*

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