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IN THIS ISSUE

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Cover
See Rafael Luque, Guobao Xu *et al.*, pp. 1210–1214. Image reproduced by permission of Guobao Xu from *Energy Environ. Sci.*, 2016, 9, 1210.



Inside cover
See Jae-Kwang Kim, Youngsik Kim *et al.*, pp. 1264–1269. Image reproduced by permission of Jae-Kwang Kim from *Energy Environ. Sci.*, 2016, 9, 1264.

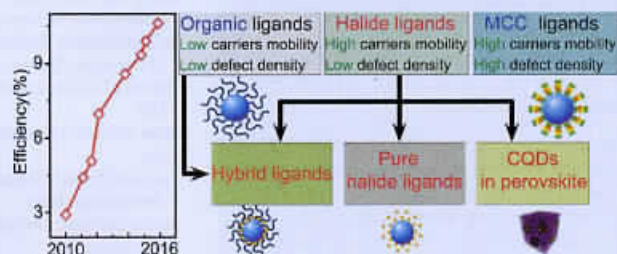
PERSPECTIVE

1130

Colloidal quantum dot ligand engineering for high performance solar cells

Ruiji Wang, Yuequn Shang, Pongsakorn Kanjanaboos, Wenjia Zhou, Zhijun Ning* and Edward H. Sargent*

Colloidal quantum dots (CQDs) are fast-improving materials for next-generation solution-processed optoelectronic devices such as solar cells, photocatalysis, light emitting diodes, and photodetectors.



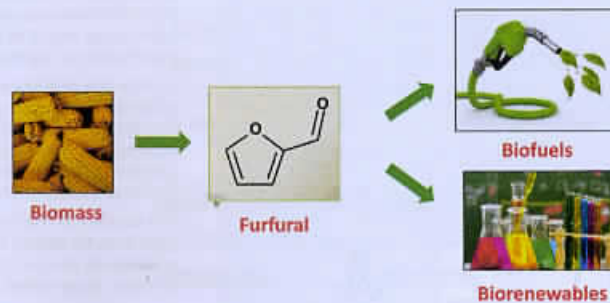
REVIEWS

1144

Furfural: a renewable and versatile platform molecule for the synthesis of chemicals and fuels

R. Mariscal, P. Maireles-Torres, M. Ojeda, I. Sádaba and M. López Granados*

The aim of this review is to discuss the most relevant chemical routes for converting furfural to chemicals and to biofuels and additives.



1190

Two-dimensional layered MoS₂: rational design, properties and electrochemical applications

Gong Zhang, Huijuan Liu,* Jiuhui Qu and Jinghong Li*

Nanostructured MoS₂ materials and their potential applications in energy conversion and storage devices.

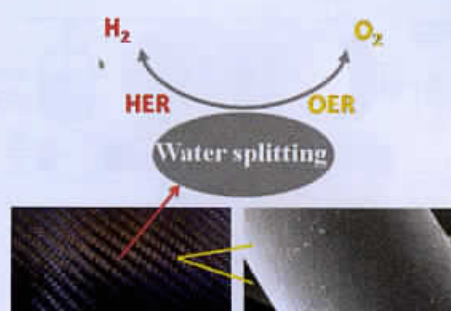
COMMUNICATIONS

1210

Unprecedented metal-free 3D porous carbonaceous electrodes for full water splitting

Jianping Lai, Suping Li, Fengxia Wu, Muhammad Saqib, Rafael Luque* and Guobao Xu*

Nitrogen, phosphorus and oxygen tri-doped porous graphite carbon@oxidized carbon cloth electrodes exhibit excellent activity and durability for full water splitting at all pH values.



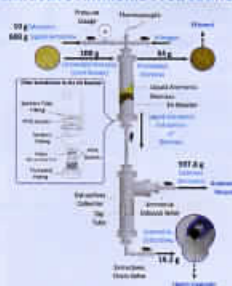
1215

Next-generation ammonia pretreatment enhances cellulosic biofuel production

L. da Costa Sousa,* M. Jin, S. P. S. Chundawat, V. Bokade, X. Tang, A. Azarpira, F. Lu, U. Avci, J. Humpala, N. Uppugundla, C. Gunawan, S. Pattathil, A. M. Cheh, N. Kothari, R. Kumar, J. Ralph, M. G. Hahn, C. E. Wyman, S. Singh, B. A. Simmons, B. E. Dale* and V. Balan*

Extractive ammonia pretreatment converts crystalline cellulose I_β to a highly digestible cellulose III₁ and selectively extracts up to ~45% of the lignin from lignocellulosic biomass with near-quantitative retention of all polysaccharides.

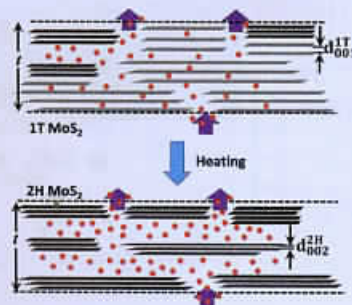
Extractive Ammonia Pretreatment



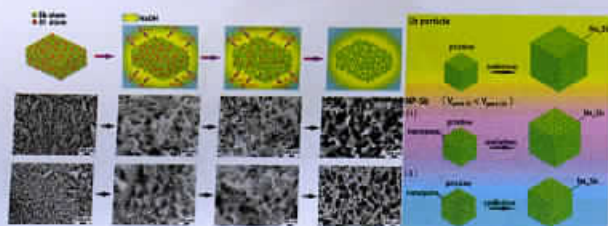
1224

High performance MoS₂ membranes: effects of thermally driven phase transition on CO₂ separation efficiency

A. Achari, Sahana S. and M. Eswaramoorthy*

MoS₂ membranes show high performance H₂/CO₂ separation at high H₂ permeability. The MoS₂ membranes were found to be thermally stable up to 160 °C and a significant increase in gas permeability was observed due to the thermally driven phase transition from the 1T to the 2H phase.

1229

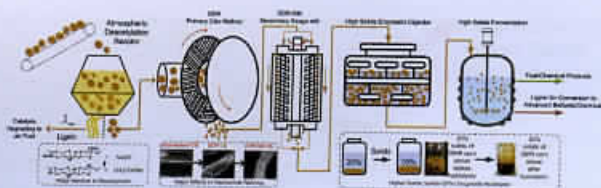


The morphology-controlled synthesis of a nanoporous-antimony anode for high-performance sodium-ion batteries

Shuai Liu, Jinkui Feng,* Xiufang Bian,* Jie Liu and Hui Xu

We propose a novel, practical way to prepare nanoporous Sb with different morphologies and Sb particles of varying size through chemical dealloying of Al–Sb alloy ribbon precursors with different compositions, a top-down process.

1237

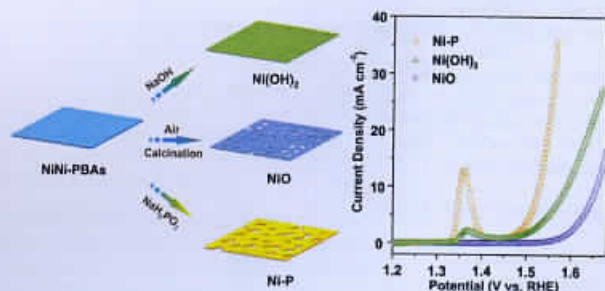


DMR (deacetylation and mechanical refining) processing of corn stover achieves high monomeric sugar concentrations (230 g L^{-1}) during enzymatic hydrolysis and high ethanol concentrations ($>10\% \text{ v/v}$) during fermentation without hydrolysate purification or concentration

Xiaowen Chen,* Erik Kuhn, Edward W. Jennings, Robert Nelson, Ling Tao, Min Zhang and Melvin P. Tucker*

Distilling and purifying ethanol is resource intensive.

1246

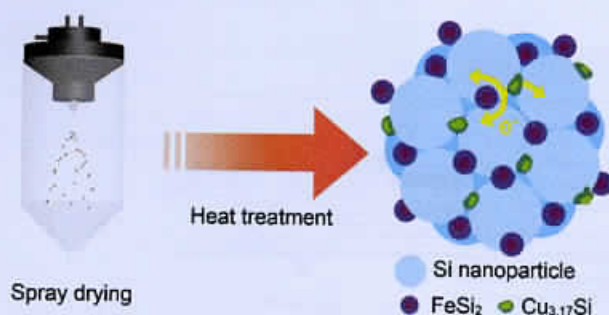


Carbon coated porous nickel phosphides nanoplates for highly efficient oxygen evolution reaction

Xin-Yao Yu, Yi Feng, Buyuan Guan, Xiong Wen (David) Lou* and Ungyu Paik*

Prussian blue analogue (PBA)-derived carbon coated porous nickel phosphides nanoplates exhibit enhanced electrocatalytic activity for oxygen evolution reaction.

1251



Micron-sized Fe–Cu–Si ternary composite anodes for high energy Li-ion batteries

Sujung Chae, Minseong Ko, Seungkyu Park, Namhyung Kim, Jiyoung Ma and Jaephil Cho*

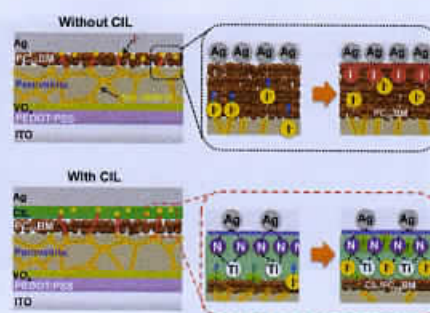
To develop a practicable Si-based anode for high-energy LIBs, a FeCuSi composite was developed by properly building Si-metal alloys.

1258

Achieving long-term stable perovskite solar cells via ion neutralization

Hyungcheol Back, Geunjin Kim, Junghwan Kim, Jaemin Kong, Tae Kyun Kim, Hongkyu Kang, Heejoo Kim, Jinho Lee, Seongyu Lee and Kwanghee Lee*

Corrosive ionic defects in perovskite films degrade perovskite solar cells (PSCs) and long-term stable PSCs are realized by neutralizing the defects.



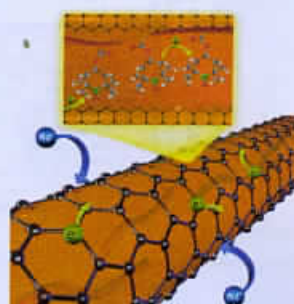
PAPERS

1264

Encapsulation of organic active materials in carbon nanotubes for application to high-electrochemical-performance sodium batteries

Jae-Kwang Kim,* Yongil Kim, Seungyoung Park, Hyunhyub Ko and Youngsik Kim*

A PTMA-impregnated CNT electrode achieves the enhancement of discharge capacity, cycleability and rate capability of sodium batteries.

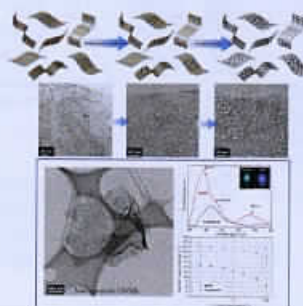


1270

Scalable fabrication of micron-scale graphene nanomeshes for high-performance supercapacitor applications

Hyun-Kyung Kim, Seong-Min Bak, Suk Woo Lee, Myeong-Seong Kim, Byeongho Park, Su Chan Lee, Yeon Jun Choi, Seong Chan Jun, Joong Tark Han, Kyung-Wan Nam, Kyung Yoon Chung, Jian Wang, Jigang Zhou, Xiao-Qing Yang, Kwang Chul Roh* and Kwang-Bum Kim*

GNM electrodes exhibit superior electrochemical properties.

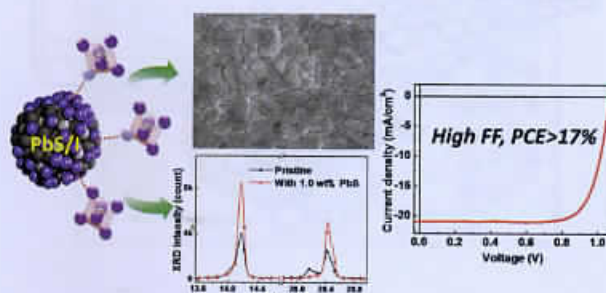


1282

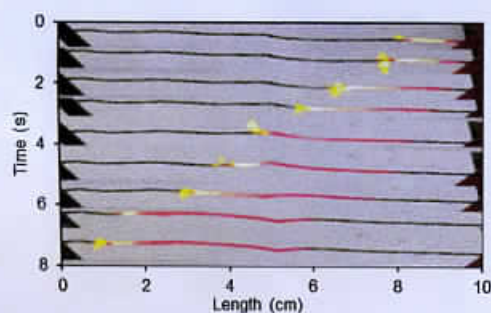
Intermixing-seeded growth for high-performance planar heterojunction perovskite solar cells assisted by precursor-capped nanoparticles

Shao-Sian Li, Chi-Huang Chang, Ying-Chiao Wang, Chung-Wei Lin, Di-Yan Wang, Jou-Chun Lin, Chia-Chun Chen, Hwo-Shuenn Sheu, Hao-Chung Chia, Wei-Ru Wu, U-Ser Jeng,* Chi-Te Liang, Raman Sankar, Fang-Cheng Chou and Chun-Wei Chen*

A novel approach to modulate the nucleation and growth of perovskite crystals by intermixing precursor-capped nanoparticles has been reported.



1290

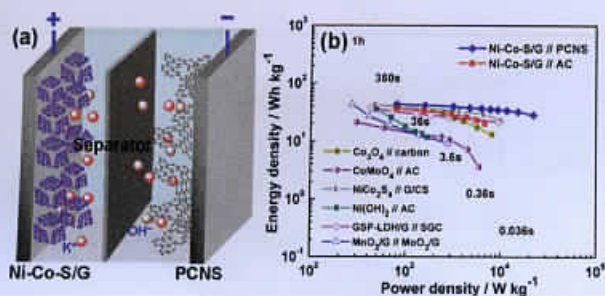


Sustainable power sources based on high efficiency thermopower wave devices

Sayalee G. Mahajan, Albert Tianxiang Liu, Anton L. Cottrill, Yuichiro Kunai, David Bender, Javier Castillo Jr, Stephen L. Gibbs and Michael S. Strano*

Thermopower wave devices are shown to achieve over 1% chemical-to-electrical conversion efficiency, producing energy densities on par with Li-ion batteries.

1299

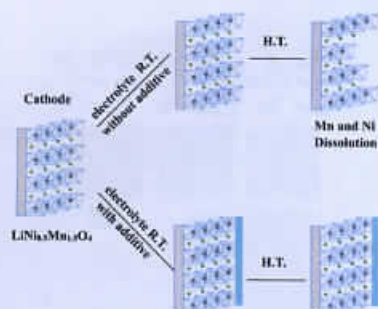


Electroactive edge site-enriched nickel–cobalt sulfide into graphene frameworks for high-performance asymmetric supercapacitors

Juan Yang, Chang Yu, Xiaoming Fan, Suxia Liang, Shaofeng Li, Huawei Huang, Zheng Ling, Ce Hao and Jieshan Qiu*

The integrated hybrid architectures composed of edge site-enriched nickel–cobalt sulfide (Ni–Co–S) nanoparticles and graphene as advanced materials for asymmetric supercapacitors are configured, delivering a superb rate capability.

1308

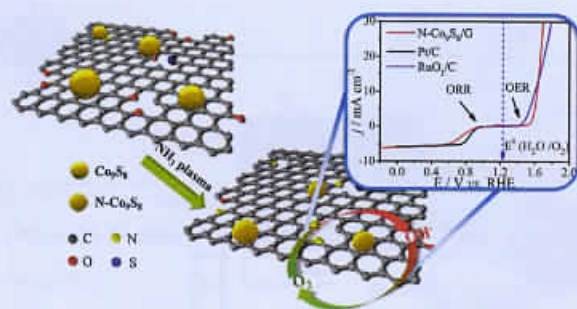


Development of novel lithium borate additives for designed surface modification of high voltage $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ cathodes

Mengqing Xu, Liu Zhou, Yingnan Dong, Yanjing Chen, Julien Demeaux, Alex D. MacIntosh, Arnd Garsuch and Brett L. Lucht*

A novel series of lithium alkyl trimethyl borates and lithium aryl trimethyl borates have been prepared and investigated as cathode film forming additives.

1320



Etched and doped Co_9S_8 /graphene hybrid for oxygen electrocatalysis

Shuo Dou, Li Tao, Jia Huo, Shuangyin Wang* and Liming Dai

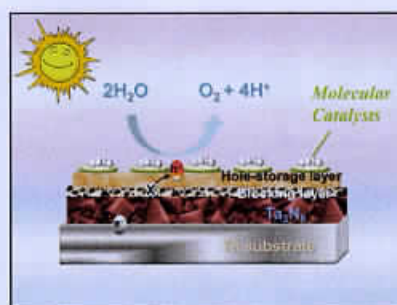
Simultaneous etching and doping of cobalt sulfides–graphene hybrid with NH_3 -plasma effectively enhances the oxygen electrocatalytic activity.

1327

Enabling an integrated tantalum nitride photoanode to approach the theoretical photocurrent limit for solar water splitting

Guiji Liu, Sheng Ye, Pengli Yan, Fengqiang Xiong, Ping Fu, Zhiliang Wang, Zheng Chen, Jingying Shi* and Can Li*

The integrated architecture enables the Ta_3N_5 photoanode to approach the theoretical photocurrent limit for solar water splitting.

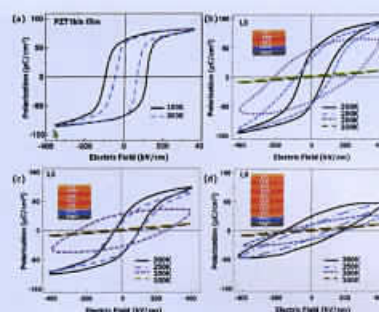


1335

Giant pyroelectric energy harvesting and a negative electrocaloric effect in multilayered nanostructures

Gaurav Vats,* Ashok Kumar, Nora Ortega, Chris R. Bowen and Ram S. Katiyar

This work examines the potential of $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3/\text{CoFe}_2\text{O}_4$ (PZT/CFO) multi-layered nanostructures (MLNs) to achieve a giant electrocaloric effect (ECE) and enhanced pyroelectric energy harvesting.

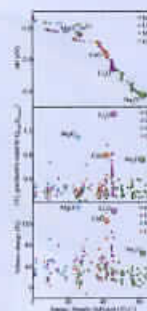


1346

Large scale computational screening and experimental discovery of novel materials for high temperature CO_2 capture

Matthew T. Dunstan, Anubhav Jain, Wen Liu, Shyue Ping Ong, Tao Liu, Jeongjae Lee, Kristin A. Persson, Stuart A. Scott, John S. Dennis and Clare P. Grey*

A combined computational and experimental methodology is developed to predict new materials that should have desirable properties for CCS looping, and then select promising candidates to experimentally validate these predictions.

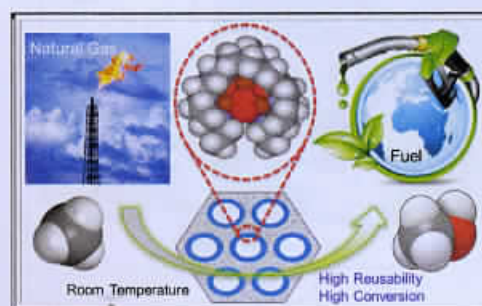


1361

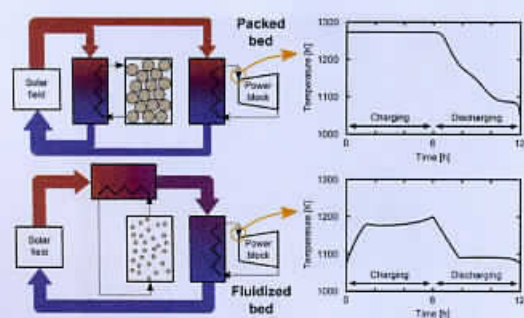
Heterogeneous formulation of the tricopper complex for efficient catalytic conversion of methane into methanol at ambient temperature and pressure

Chih-Cheng Liu, Chung-Yuan Mou, Steve S.-F. Yu and Sunney I. Chan*

The development of a heterogeneous catalyst capable for efficient selective conversion of methane into methanol with multiple turnovers under ambient conditions is reported here.



1375

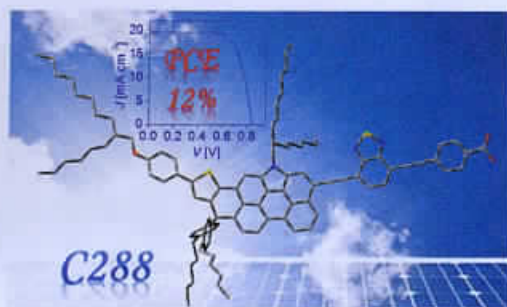


The effect of the gas–solid contacting pattern in a high-temperature thermochemical energy storage on the performance of a concentrated solar power plant

S. Ströhle, A. Haselbacher,* Z. R. Jovanovic and A. Steinfeld

This work presents a framework for comparing reactor concepts for thermochemical storage and analyzing their impact on the performance of CSP plants.

1390

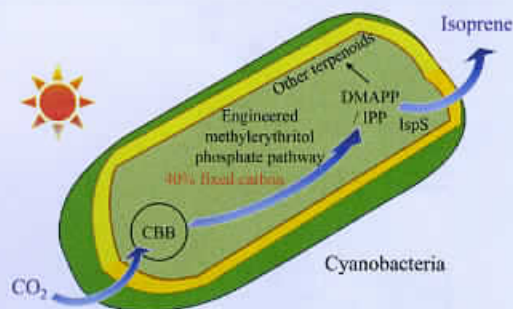


Improving the performance of dye-sensitized solar cells with electron-donor and electron-acceptor characteristic of planar electronic skeletons

Yameng Ren, Yang Li, Shu Chen, Jiao Liu, Jing Zhang and Peng Wang*

Dye C288 with an almost planar electronic skeleton achieved an excellent PCE of 12%.

1400

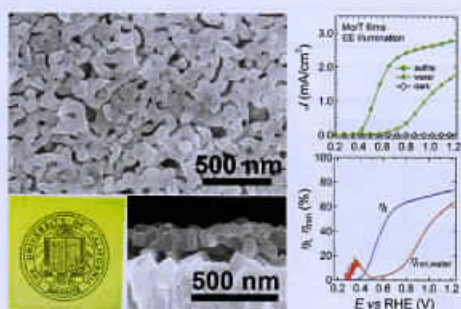


Engineering the methylerythritol phosphate pathway in cyanobacteria for photosynthetic isoprene production from CO₂

Xiang Gao, Fang Gao, Deng Liu, Hao Zhang, Xiaoqun Nie and Chen Yang*

The methylerythritol phosphate pathway in photosynthetic cyanobacteria was engineered to allow highly efficient production of isoprene from CO₂.

1412



Textured nanoporous Mo:BiVO₄ photoanodes with high charge transport and charge transfer quantum efficiencies for oxygen evolution

Vineet Nair, Craig L. Perkins, Qiying Lin and Matt Law*

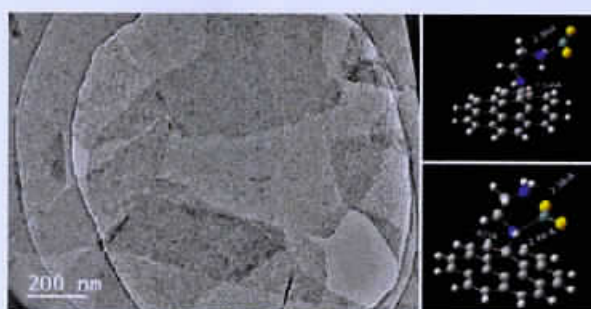
Nanoporous, catalyst-free BiVO₄ films made by a simple spin coating process show a hole-limited charge transport quantum efficiency of ~70% and >60% charge transfer efficiency for oxidizing water.

1430

Enhancing the cycling stability of Na-ion batteries by bonding SnS₂ ultrafine nanocrystals on amino-functionalized graphene hybrid nanosheets

Yong Jiang, Min Wei, Jinkui Feng, Yuchen Ma and Shenglin Xiong*

An integrated composite tin sulfide bonded on an amino-functionalized graphene as a novel anode material for NIBs is reported. Tight contact with SnS₂ nanocrystals and discharge products on the amino-functionalized graphene interface results in excellent electrochemical performance.

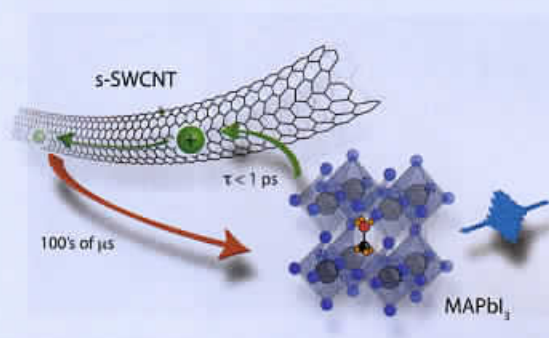


1439

Efficient charge extraction and slow recombination in organic–inorganic perovskites capped with semiconducting single-walled carbon nanotubes

Rachelle Ihly, Anne-Marie Dowgiallo, Mengjin Yang, Philip Schulz, Noah J. Stanton, Obadiah G. Reid, Andrew J. Ferguson, Kai Zhu, Joseph J. Berry and Jeffrey L. Blackburn*

Capping perovskite absorber layers with semiconducting carbon nanotubes enables sub-picosecond hole extraction and recombination times of hundreds of microseconds.

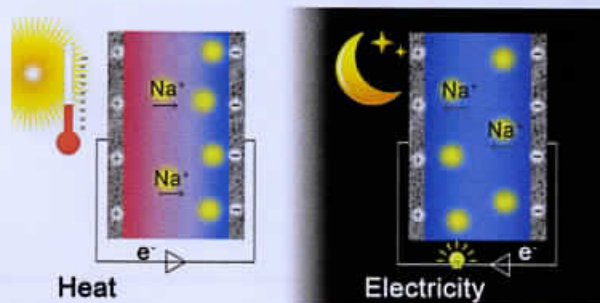


1450

Ionic thermoelectric supercapacitors

D. Zhao, H. Wang, Z. U. Khan, J. C. Chen, R. Gabrielsson, M. P. Jonsson, M. Berggren and X. Crispin*

Ionic thermoelectric supercapacitor: charged by heat during the day and discharged at night.

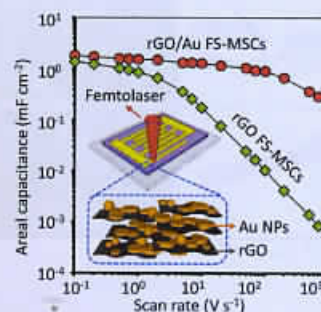


1458

High-rate in-plane micro-supercapacitors scribed onto photo paper using *in situ* femtolaser-reduced graphene oxide/Au nanoparticle microelectrodes

R.-Z. Li, Rui Peng, K. D. Kihm, S. Bai, D. Bridges, U. Tumuluri, Z. Wu, T. Zhang,* G. Compagnini, Z. Feng and A. Hu*

Direct laser-reduction of graphene oxide (GO), as a lithography-free approach, has been proven effective in manufacturing in-plane micro-supercapacitors (MSCs) with fast ion diffusion.



1468



Novel porous molybdenum tungsten phosphide hybrid nanosheets on carbon cloth for efficient hydrogen evolution

Xu-Dong Wang, Yang-Fan Xu, Hua-Shang Rao, Wei-Jian Xu, Hong-Yan Chen, Wei-Xiong Zhang, Dai-Bin Kuang* and Cheng-Yong Su

Owing to the 3D scaffolds, porous nanosheets, and strong synergistic effect of Mo and W atoms, the Mo–W–P hybrid behaves as an efficient electrocatalyst for the hydrogen evolution reaction.

1476

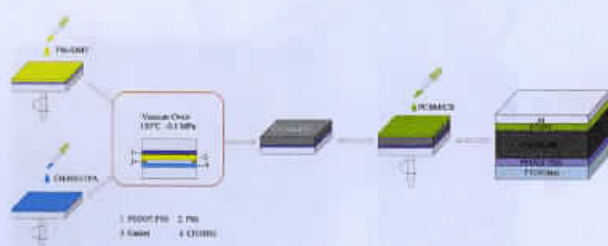


Can slow-moving ions explain hysteresis in the current–voltage curves of perovskite solar cells?

Giles Richardson,* Simon E. J. O’Kane, Ralf G. Niemann, Timo A. Peltola, Jamie M. Foster, Petra J. Cameron and Alison B. Walker*

We have developed a charge transport model that explicitly accounts for ion migration. This model has been used to interpret measured current–voltage characteristics that show hysteresis.

1486

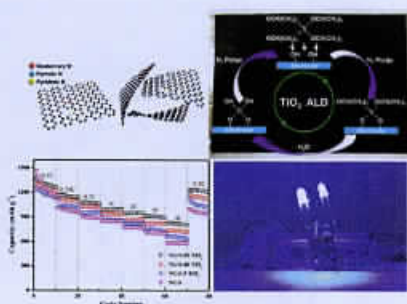


The growth of a $\text{CH}_3\text{NH}_3\text{PbI}_3$ thin film using simplified close space sublimation for efficient and large dimensional perovskite solar cells

Qiang Guo, Cong Li, Wenyuan Qiao, Shuang Ma, Fuzhi Wang, Bing Zhang, Linhua Hu, Songyuan Dai* and Zhan’ao Tan*

We demonstrate a novel simplified close space sublimation (CSS) deposition for growing a high quality $\text{CH}_3\text{NH}_3\text{PbI}_3$ thin film in a low-vacuum and even non-vacuum oven.

1495



Atomic layer deposited TiO_2 on a nitrogen-doped graphene/sulfur electrode for high performance lithium–sulfur batteries

Mingpeng Yu,* Junsheng Ma, Hongquan Song, Aiji Wang, Fuyang Tian, Yinshu Wang, Hong Qiu and Rongming Wang

A nitrogen-doped graphene/sulfur composite was further modified with atomic layers of TiO_2 and used as the cathode of lithium–sulfur batteries, exhibiting superior cycling stability, good rate capability and high coulombic efficiency.

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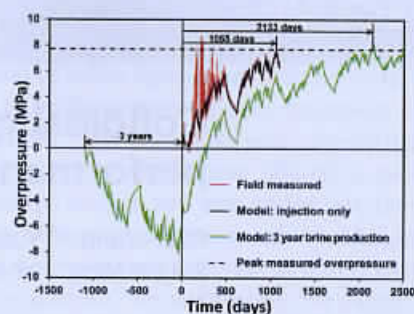
Mohar

1504

Managing geologic CO₂ storage with pre-injection brine production: a strategy evaluated with a model of CO₂ injection at Snøhvit

Thomas A. Buscheck,* Joshua A. White, Susan A. Carroll, Jeffrey M. Bielicki and Roger D. Aines

By removing brine from a reservoir prior to storing CO₂, storage capacity can be increased by nearly an equivalent volume.



CORRECTION

1513

Correction: 2D phosphorene as a water splitting photocatalyst: fundamentals to applications

Mohammad Ziur Rahman, Chi Wai Kwong, Kenneth Davey and Shi Zhang Qiao*