

Energy & Environmental Science

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IN THIS ISSUE

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Inside cover
See Kaiming Deng,
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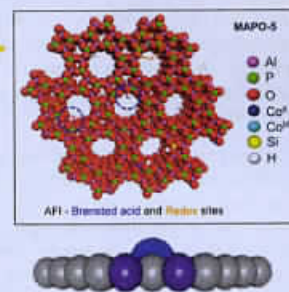
PERSPECTIVE

687

Some of tomorrow's catalysts for processing renewable and non-renewable feedstocks, diminishing anthropogenic carbon dioxide and increasing the production of energy

John Meurig Thomas* and Kenneth D. M. Harris*

A wide-ranging overview is presented of the likely impact that heterogeneous catalytic systems will play in tackling some critically important societal and environmental issues in the future.



REVIEWS

709

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

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

In this review, we focus on analysing the fundamental electronic, optical and chemical properties of 2D phosphorene to assess its suitability as a metal-free water splitting photocatalyst.

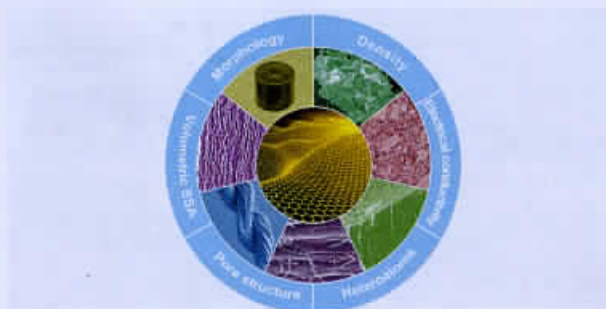


729

Carbon materials for high volumetric performance supercapacitors: design, progress, challenges and opportunities

Qian Wang, Jun Yan* and Zhuangjun Fan*

This review summarizes recent progress in the design and fabrication of carbon materials for high volumetric performance supercapacitors.

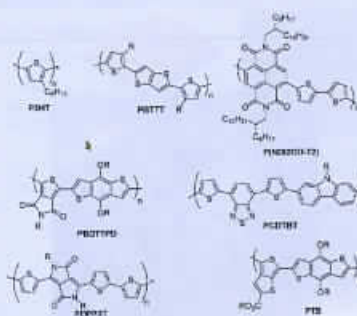


763

Current methodologies for a sustainable approach to π -conjugated organic semiconductors

Assunta Marrocchi,* Antonio Facchetti, Daniela Lanari, Chiara Petrucci and Luigi Vaccaro*

The development of waste minimized and clean synthetic methodologies to afford polymeric semiconductors is essential for the successful commercialization of opto-electronic devices.



ANALYSIS

787

Wells to wheels: water consumption for transportation fuels in the United States

David J. Lampert,* Hao Cai and Amgad Elgowainy

Supply chains for transportation fuels were analyzed using an extensive system boundary to gain insights into the connections between transportation energy and water resource consumption.

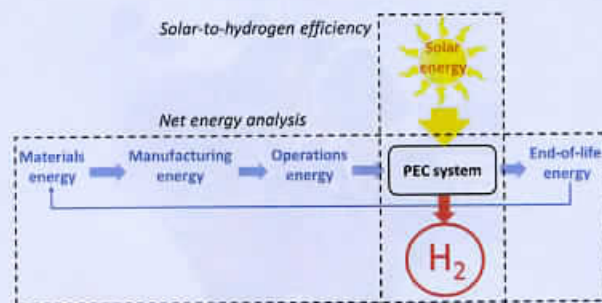


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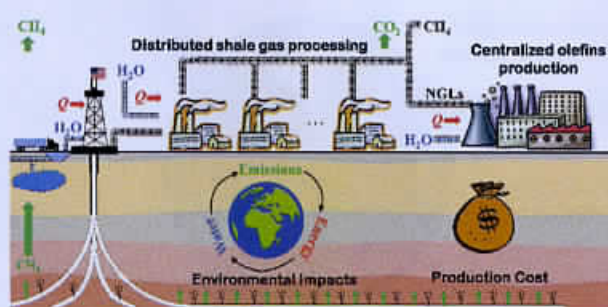
Opportunities to improve the net energy performance of photoelectrochemical water-splitting technology

Roger Sathre,* Jeffery B. Greenblatt,* Karl Walczak, Ian D. Sharp, John C. Stevens, Joel W. Ager, III and Frances A. Houle

The hydrogen energy provided by solar-driven photoelectrochemical water splitting must be greater than the energy used to produce and operate the technology, to enable energetic benefits to society.



820



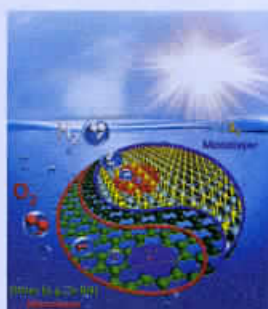
Deciphering the true life cycle environmental impacts and costs of the mega-scale shale gas-to-olefins projects in the United States

Chang He and Fengqi You*

Using detailed techno-economic-environmental models, we investigate the environmental impacts and production costs of the mega-scale shale gas-to-olefins projects in the U.S.

COMMUNICATIONS

841



Efficient band structure tuning, charge separation, and visible-light response in ZrS₂-based van der Waals heterostructures

Xirui Zhang, Zhaoshun Meng, Dewei Rao, Yunhui Wang, Qi Shi, Yuzhen Liu, Haiping Wu, Kaiming Deng,* Hongyang Liu* and Ruifeng Lu*

Bilayer ZrS₂-based vdW heterostructures are proposed as efficient photocatalysts for water splitting under visible light.

850



Facet-controlled hollow Rh₂S₃ hexagonal nanoprisms as highly active and structurally robust catalysts toward hydrogen evolution reaction

Donghwan Yoon, Bora Seo, Jaeyoung Lee, Kyoung Sik Nam, Byeongyoon Kim, Suhyun Park, Hionsuck Baik, Sang Hoon Joo* and Kwangyeol Lee*

Hollow Rh₂S₃ hexagonal nanoprisms, prepared by one-step formation of core-shell nanoprisms followed by the etching of a core, exhibit very high catalytic activity and excellent stability toward hydrogen evolution reaction.

857



Incineration of organic solar cells: efficient end of life management by quantitative silver recovery

Roar R. Søndergaard,* Yannick-Serge Zimmermann, Nieves Espinosa, Markus Lenz and Frederik Krebs

Silver from the electrodes of 1 m² organic solar cells was quantitatively recovered by acid extraction from incineration ashes.

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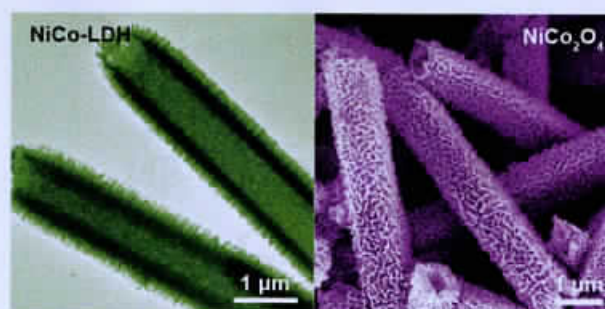
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Self-supported formation of hierarchical NiCo₂O₄ tetragonal microtubes with enhanced electrochemical properties

Fei-Xiang Ma, Le Yu, Cheng-Yan Xu and Xiong Wen (David) Lou*

Hierarchical NiCo₂O₄ tetragonal microtubes prepared by a self-supported chemical transformation process exhibit an excellent electrochemical performance.

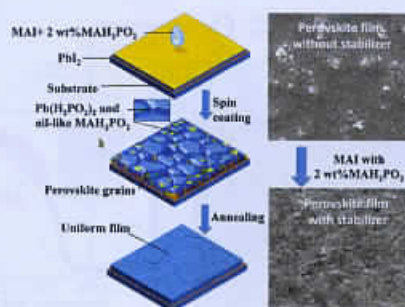


867

Unraveling the hidden function of a stabilizer in a precursor in improving hybrid perovskite film morphology for high efficiency solar cells

Zhengguo Xiao, Dong Wang, Qingfeng Dong,* Qi Wang, Wei Wei, Jun Dai, Xiaocheng Zeng and Jinsong Huang*

The precursor purity is critical for the perovskite film morphology and solar cell device performance.

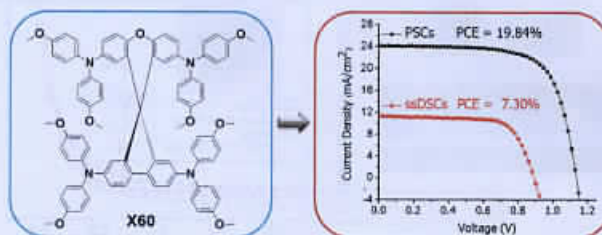


873

A low-cost spiro[fluorene-9,9'-xanthene]-based hole transport material for highly efficient solid-state dye-sensitized solar cells and perovskite solar cells

Bo Xu, Dongqin Bi, Yong Hua, Peng Liu, Ming Cheng, Michael Grätzel, Lars Kloo, Anders Hagfeldt* and Licheng Sun*

A low-cost spiro[fluorene-9,9'-xanthene]-based HTM termed **X60** showed high PCEs of 7.30% in ssDSCs and 19.84% in PSCs under one sun, respectively.

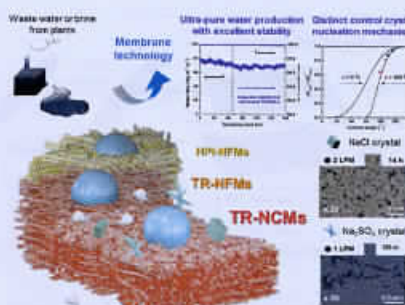


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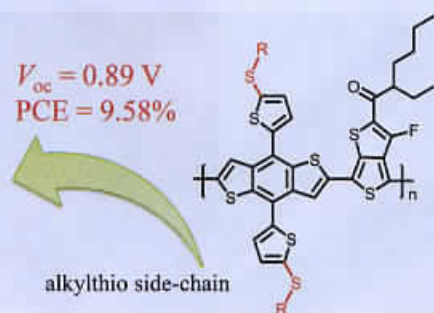
Thermally rearranged polymer membranes for desalination

Ji Hoon Kim, Sang Hyun Park, Moon Joo Lee, Sang Min Lee, Won Hyo Lee, Kang Hyuck Lee, Na Rae Kang, Hye Jin Jo, Jeong F. Kim, Enrico Drioli* and Young Moo Lee*

Thermally rearranged polybenzoxazole-co-imide (TR-PBOI) membranes exhibited excellent flux ($80 \text{ kg m}^{-2} \text{ h}^{-1}$) and salt rejection (>99.99%) over more than 186 hours as well as potential for use in membrane crystallization.



885

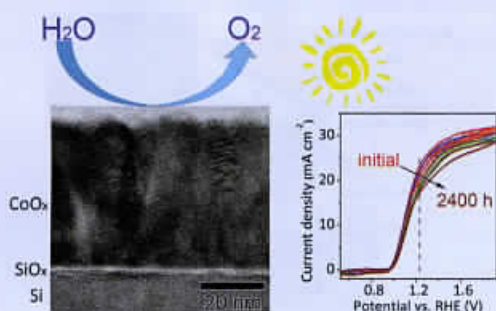


High-performance polymer solar cells based on a 2D-conjugated polymer with an alkylthio side-chain

Chaohua Cui, Zhicai He,* Yue Wu, Xiao Cheng, Hongbin Wu, Yongfang Li,* Yong Cao and Wai-yeung Wong*

The inverted-structured PSC based on **PBDTT-S-TT-CF** exhibited a high PCE of 9.58% with a remarkably high V_{oc} of 0.89 V.

892

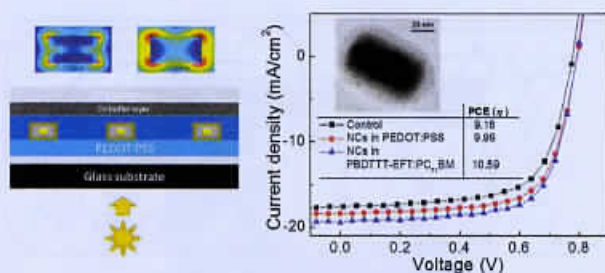


570 mV photovoltage, stabilized n-Si/CoO_x heterojunction photoanodes fabricated using atomic layer deposition

Xinghao Zhou, Rui Liu, Ke Sun, Kimberly M. Papadantonakis, Bruce S. Brunschwig and Nathan S. Lewis*

Deposition of a 50 nm thick CoO_x layer on planar n-Si yields stable, high-performance photoanodes for water oxidation.

898

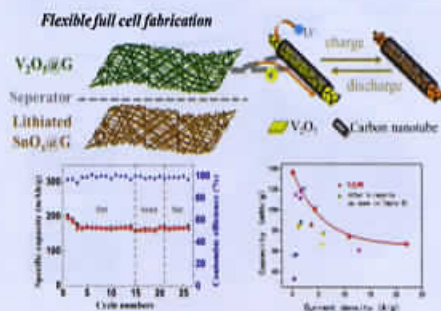


Au/Ag core-shell nanocuboids for high-efficiency organic solar cells with broadband plasmonic enhancement

Shenghua Liu, Ruibin Jiang, Peng You, Xingzhong Zhu, Jianfang Wang and Feng Yan*

We introduced Au@Ag core-shell nanocuboids with broadband plasmonic enhancement in organic photovoltaics, which show multimode localized surface plasmon resonance that can be tuned to match the light absorption spectra of the devices by changing the geometric size.

906



Encapsulating V₂O₅ into carbon nanotubes enables the synthesis of flexible high-performance lithium ion batteries

Debin Kong, Xianglong Li, Yunbo Zhang, Xiao Hai, Bin Wang, Xiongying Qiu, Qi Song, Quan-Hong Yang* and Linjie Zhi*

A facile synthesis of high performance flexible V₂O₅-based cathodes constructed by V₂O₅ nanosheets encapsulated within multi-graphene nanotubes and the successful demonstration of a flexible full cell.

912

Highly efficient organic photovoltaic cells based on a novel donor-acceptor polymer

Fei Zhao, Liangti Qiu

A high performance polymer solar cell was developed directly on the basis of the novel donor-acceptor polymer with an open circuit voltage (PCE),

917

A redox flow battery with a novel organic redox couple

Qizhao Li, and Qin

Charge/discharge cycle life of a Li-I redox flow battery with a high current density of

PAPER

922

Enhanced performance of organic solar cells by using a novel polymer

Norman David K

Hybrid organic-inorganic solar cells with a carbon nanotube pathway upon

932

Universal hole transport layer for organic photovoltaic cells

Kyung Yabing

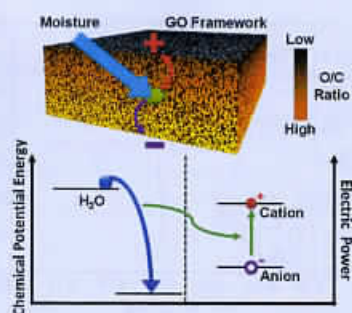
Tailoring the structure of organic perovskite solar cells with an open circuit voltage (PCE),

912

Highly efficient moisture-enabled electricity generation from graphene oxide frameworks

Fei Zhao, Yuan Liang, Huhu Cheng, Lan Jiang and Liangti Qu*

A high performance chemical potential energy harvester for directly generating electric power has been developed on the basis of the three-dimensional assembly of graphene oxide with an oxygen gradient.

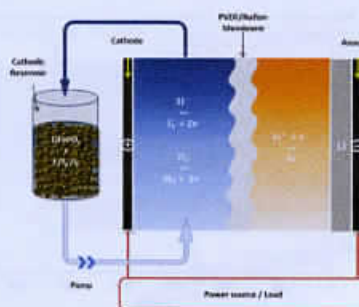


917

A redox flow lithium battery based on the redox targeting reactions between LiFePO_4 and iodide

Qizhao Huang, Jing Yang, Chee Boon Ng, Chuankun Jia and Qing Wang*

Charge/discharge LiFePO_4 with a single redox species: a Li-I redox flow lithium battery with strikingly high energy density for large-scale energy storage applications.



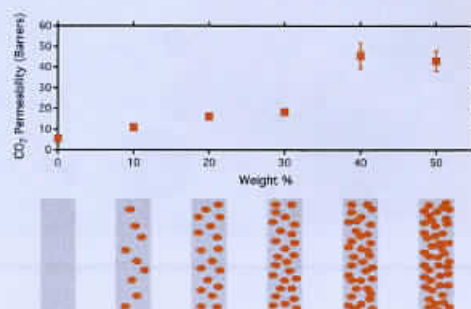
PAPERS

922

Enhanced permeation arising from dual transport pathways in hybrid polymer–MOF membranes

Norman C. Su, Daniel T. Sun, Christine M. Beavers, David K. Britt, Wendy L. Queen and Jeffrey J. Urban*

Hybrid polymer/inorganic membranes with dual transport pathways exhibit exceptional separation performance for carbon capture and non-classical gas transport behavior upon formation of a percolative network.

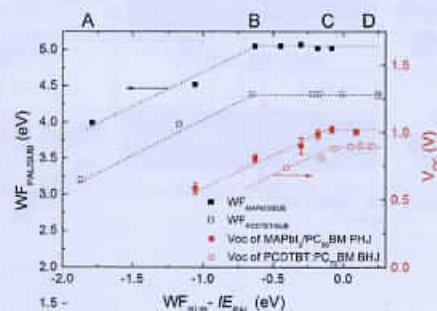


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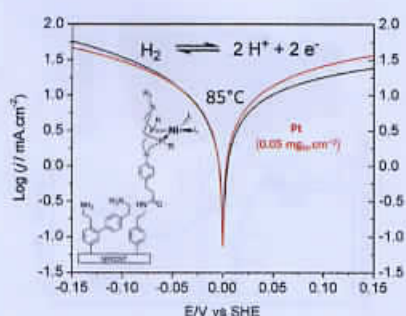
Universal energy level tailoring of self-organized hole extraction layers in organic solar cells and organic–inorganic hybrid perovskite solar cells

Kyung-Geun Lim, Soyeong Ahn, Young-Hoon Kim, Yabing Qi and Tae-Woo Lee*

Tailoring the interface energetics between a polymeric hole extraction layer (HEL) and a photoactive layer (PAL) in organic photovoltaics (OPVs) and organic–inorganic hybrid perovskite solar cells (PrSCs) is very important to maximize open circuit voltage (V_{oc}), power conversion efficiency (PCE), and device lifetime.



940

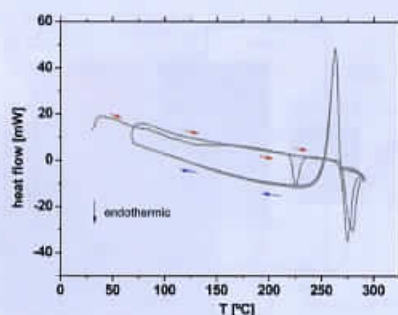


Bio-inspired noble metal-free nanomaterials approaching platinum performances for H₂ evolution and uptake

Tran N. Huan, Reuben T. Jane, Anass Benayad, Laure Guetaz, Phong D. Tran and Vincent Artero*

3D structuring of the electrode boosts the performances of molecular-engineered nanomaterials based on bio-inspired nickel-diphosphine catalysts operating at the thermodynamic equilibrium in PEMFC relevant conditions.

948

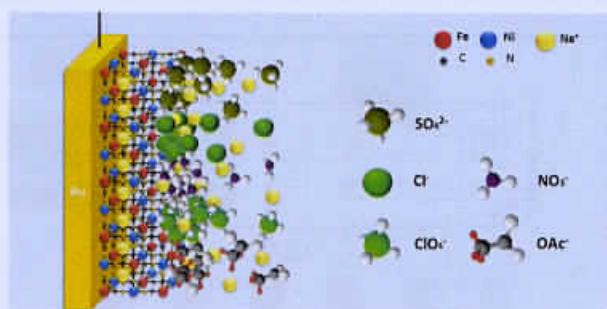


Glass-amorphous alkali-ion solid electrolytes and their performance in symmetrical cells

M. Helena Braga,* Andrew J. Murchison, Jorge A. Ferreira, Preetam Singh and John B. Goodenough*

Precursors of the crystalline antiperovskites $A_{3-x}H_xOCl$ ($A = \text{Li}$ or Na and $0 < x < 1$) can be rendered glass/amorphous solid Li^+ or Na^+ electrolytes by the addition of water to its solvation limit with/without the addition of a small amount of an oxide or hydroxide.

955

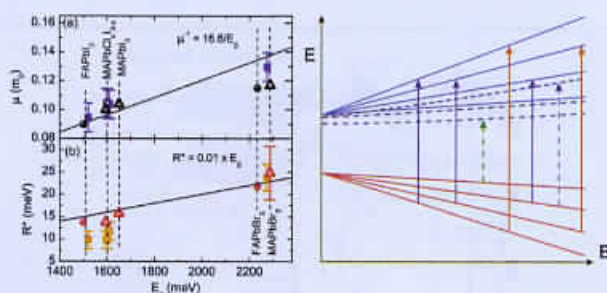


How simple are the models of Na intercalation in aqueous media?

Jeongsik Yun, Jonas Pfisterer and Aliaksandr S. Bandarenka*

This work reveals a three-stage mechanism of Na intercalation into one of the state-of-the-art battery electrode materials operating in aqueous electrolytes.

962



Determination of the exciton binding energy and effective masses for methylammonium and formamidinium lead tri-halide perovskite semiconductors

Krzysztof Galkowski, Anatolie Mitioglu, Atsuhiko Miyata, Paulina Plochocka, Oliver Portugall, Giles E. Eperon, Jacob Tse-Wei Wang, Thomas Stergiopoulos, Samuel D. Stranks, Henry J. Snaith and Robin J. Nicholas*

The reduced effective mass (μ) and excitonic Rydberg (R^*) are measured by magneto-optics for new perovskite semiconductors.

971

Calcium decarboxylation

David P. Carbon (ES) systems fossil-fueled

984

The interfacial high-energy

M. Saub M.-L. D. This paper the anionic using co-interaction based on

992

A layered sulfur

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CO₂ capture plasma problems

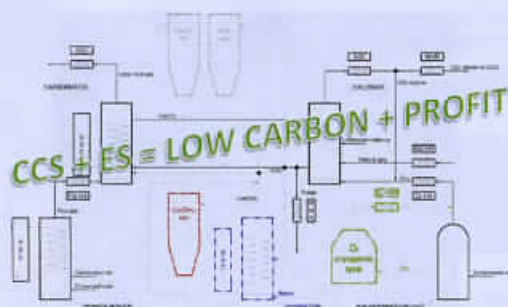
R. Snow and A. For the computational CO₂ sp

971

Calcium looping with inherent energy storage for decarbonisation of coal-fired power plant

Dawid P. Hanak,* Chechet Biliyok and Vasilije Manovic*

Carbon capture and storage (CCS) with energy storage (ES) systems increase flexibility and profitability of fossil-fuel-fired power systems.

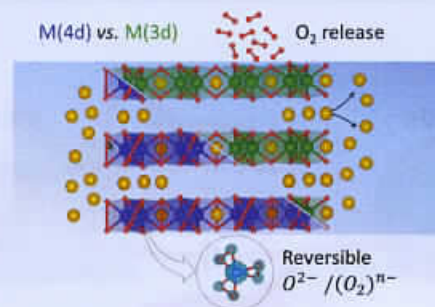


984

The intriguing question of anionic redox in high-energy density cathodes for Li-ion batteries

M. Saubanère, E. McCalla, J.-M. Tarascon and M.-L. Doublet*

This paper aims to identify robust descriptors to rationalize the anionic redox mechanism in layered Li-rich TM-oxides using conceptual tools, such as atomic charges, orbital interactions and crystal orbital overlap populations (COOP), based on first-principles DFT calculations.

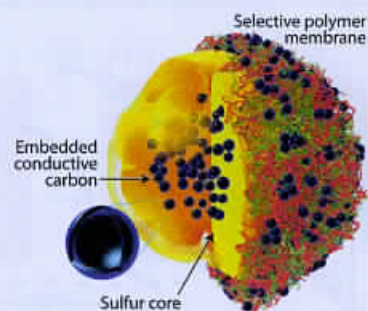


992

A layer-by-layer supramolecular structure for a sulfur cathode

Claudiu B. Bucur, John Muldoon* and Adrian Lita

The anatomy of a truffle inspired sulfur particle for a battery cathode.

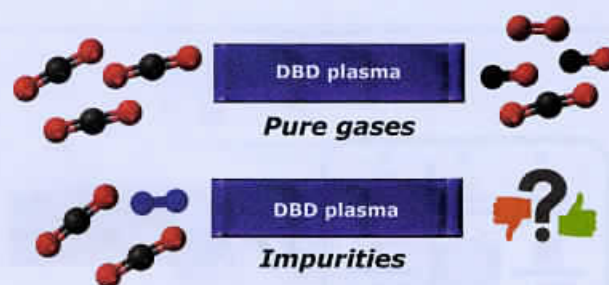


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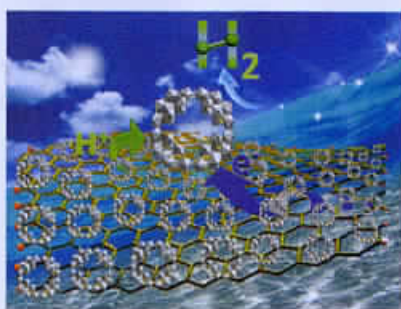
CO₂ conversion in a dielectric barrier discharge plasma: N₂ in the mix as a helping hand or problematic impurity?

R. Snoeckx,* S. Heijkens, K. Van Wesenbeeck, S. Lenaerts and A. Bogaerts

For the first time an extensive experimental and computational study was performed on the effect of N₂ on CO₂ splitting in a dielectric barrier discharge plasma.



1012

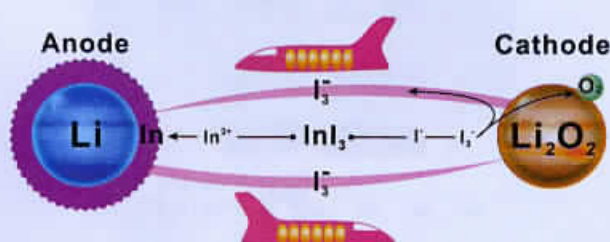


Enhanced proton and electron reservoir abilities of polyoxometalate grafted on graphene for high-performance hydrogen evolution

Rongji Liu, Guangjin Zhang,* Hongbin Cao, Suojiang Zhang, Yongbing Xie, Ali Haider, Ulrich Kortz,* Banghao Chen, Naresh S. Dalal,* Yongsheng Zhao, Linjie Zhi, Cai-Xia Wu, Li-Kai Yan,* Zhongmin Su and Bineta Keita

A 3D configuration of high-quality graphene sheets and a polyoxometalate $[H_7P_8W_{48}O_{184}]^{33-}$ showing excellent hydrogen evolution activity at extremely low overpotential.

1024

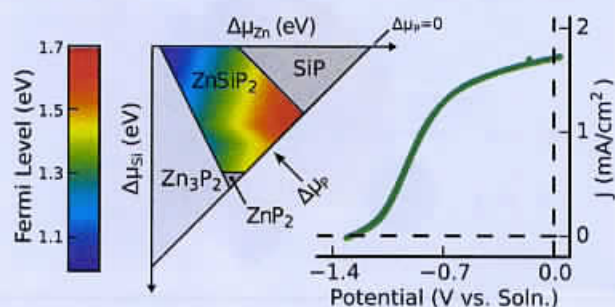


A self-defense redox mediator for efficient lithium–O₂ batteries

Tao Zhang, Kaiming Liao, Ping He and Haoshen Zhou*

InI_3 , a self-defense redox mediator, can form a pre-deposited indium layer to resist the synchronous attack on a Li anode by the soluble I_3^- , and hence can suppress the shuttle effect in lithium–O₂ batteries.

1031



Solar energy conversion properties and defect physics of ZnSiP₂

A. D. Martinez, E. L. Warren, P. Gorai, K. A. Borup, D. Kuciauskas, P. C. Dippo, B. R. Ortiz, R. T. Macaluso, S. D. Nguyen, A. L. Greenaway, S. W. Boettcher, A. G. Norman, V. Stevanović, E. S. Toberer and A. C. Tamboli*

ZnSiP₂ is a promising candidate for lattice-matched tandem photovoltaics on silicon. Here, we explore the defect physics, luminescence, and photoelectrochemical performance of this potential top cell material.

1042



Transforming biomass conversion with ionic liquids: process intensification and the development of a high-gravity, one-pot process for the production of cellulosic ethanol

Feng Xu, Jian Sun, N. V. S. N. Murthy Konda, Jian Shi, Tanmoy Dutta, Corinne D. Scown, Blake A. Simmons and Seema Singh*

Producing concentrated sugars and minimizing water usage are key elements in the economics and environmental sustainability of advanced biofuels.

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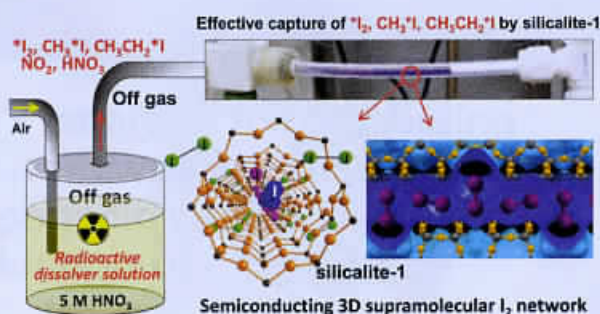
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Capture of iodine and organic iodides using silica zeolites and the semiconductor behaviour of iodine in a silica zeolite

Tung Cao Thanh Pham, Son Docao, In Chul Hwang, Mee Kyung Song, Do Young Choi, Dohyun Moon, Peter Oleynikov and Kyung Byung Yoon*

During the reprocessing of spent nuclear fuel rods, a highly moist off-gas mixture containing various volatile radioactive species, such as iodine (I_2), organic iodides and nitric acid, is produced.



1063

Harnessing low energy photons (635 nm) for the production of H_2O_2 using upconversion nanohybrid photocatalysts

Hyoung-il Kim, Oh Seok Kwon, Sujeong Kim, Wonyong Choi* and Jae-Hong Kim*

This study demonstrates, for the first time in literature, *in situ* photocatalytic synthesis of hydrogen peroxide (H_2O_2) through sensitized triplet-triplet annihilation (TTA) upconversion (UC) of low-energy, sub-bandgap photons.

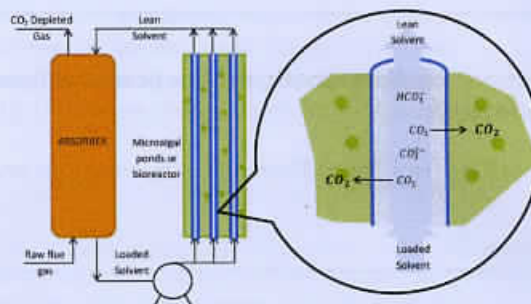


1074

Energy efficient transfer of carbon dioxide from flue gases to microalgal systems

Qi Zheng, Gregory J. O. Martin and Sandra E. Kentish*

Transfer of CO_2 directly from a capture solvent to microalgae via hollow fibre membranes, reduces energy demand and increases production.

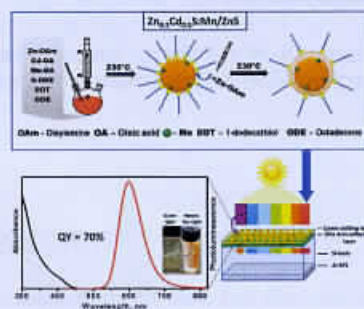


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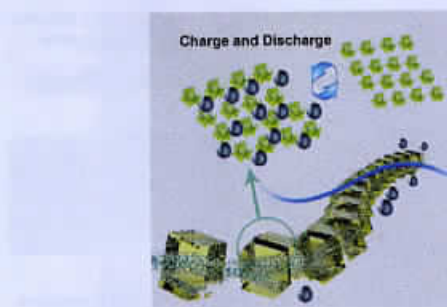
Industrially scalable and cost-effective Mn^{2+} doped $Zn_xCd_{1-x}S/ZnS$ nanocrystals with 70% photoluminescence quantum yield, as efficient down-shifting materials in photovoltaics

I. Levchuk, C. Würth, F. Krause, A. Osvet, M. Batentschuk,* U. Resch-Genger,* C. Kolbeck, P. Herre, H. P. Steinrück, W. Peukert and C. J. Brabec

We present colloiddally stable and highly luminescent $Zn_xCd_{1-x}S:Mn/ZnS$ core-shell nanocrystals (NCs) as cost-effective light converters for silicon photovoltaic (PV).



1095

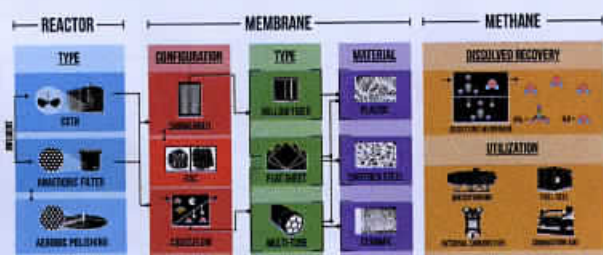


“Wiring” redox-active polyoxometalates to carbon nanotubes using a sonication-driven periodic functionalization strategy

Jun Hu, Yuanchun Ji, Wei Chen, Carsten Streb* and Yu-Fei Song*

A universal one-step strategy for the periodic deposition of redox-active polyoxometalate nanocrystals on single-walled carbon nanotubes is reported, giving access to high-performance electrodes for lithium-ion batteries.

1102



Design of anaerobic membrane bioreactors for the valorization of dilute organic carbon waste streams

Brian D. Shoener, Cheng Zhong, Anthony D. Greiner, Wendell O. Khunjar, Pei-Ying Hong and Jeremy S. Guest*

Aqueous waste organics are an abundant resource generated continuously by industry and human metabolism.

CORRECTIONS

1113

Correction: Photosynthetic production of ethanol from carbon dioxide in genetically engineered cyanobacteria

Zhengxu Gao, Hui Zhao, Zhimin Li, Xiaoming Tan and Xuefeng Lu*

1114

Correction: Selective CO production by Au coupled ZnTe/ZnO in the photoelectrochemical CO₂ reduction system

Youn Jeong Jang, Ji-Wook Jang, Jaehyuk Lee, Ju Hun Kim, Hiromu Kumagai, Jinwoo Lee, Tsutomu Minegishi, Jun Kubota, Kazunari Domen and Jae Sung Lee*