# **Energy & Environmental Science**

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#### IN THIS ISSUE

ISSN 1754-5692 CODEN EESNBY 9(7) 2161-2472 (2016)



#### Cover

See Jinlong Gong et al., pp. 2177–2196. Image reproduced by permission of Jinlong Gong from Energy Environ. Sci., 2016, 9, 2177.



#### Inside cover

See Taiho Park et al., pp. 2326–2333. Image reproduced by permission of Taiho Park from Energy Environ. Sci., 2016, 9, 2326.

#### OPINION

#### 2172

Aspects of science and technology in support of legal and policy frameworks associated with a global carbon emissions-control regime

Nathan S. Lewis

The resolution of the delegates to COP21 in Paris suggests a step toward a global carbon emissions-control regime. We explore technical aspects of such a regime, e.g., monitoring of regional  $CO_2$  emissions and control and regulation of global temperatures.



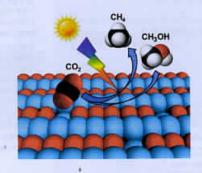
# REVIEWS

#### 2177

CO<sub>2</sub> photo-reduction: insights into CO<sub>2</sub> activation and reaction on surfaces of photocatalysts

Xiaoxia Chang, Tuo Wang and Jinlong Gong\*

This review describes the current understanding of  $CO_2$  photoreduction on the surface of heterogeneous catalysts with a particular focus on the reaction mechanism and pathways as well as the adsorption/activation of  $CO_2$ .

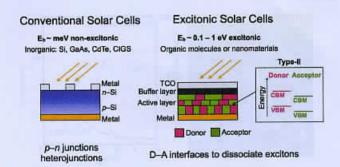


#### 2197

# Computer calculations across time and length scales in photovoltaic solar cells

Marco Bernardi\* and Jeffrey C. Grossman\*

Photovoltaic (PV) solar cells convert solar energy to electricity through a cascade of microscopic processes spanning over 10 order of magnitudes of time and length. We review the computational methods available to study PV solar cells, focusing on recent advances and open problems.



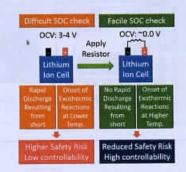
#### PERSPECTIVE

#### 2219

### Opportunities for near zero volt storage of lithium ion batteries

K. R. Crompton and B. J. Landi\*

There are inherent safety risks associated with inactive lithium ion batteries leading to greater restrictions and regulations on shipping and inactive storage. Near zero volt storage under fixed load of all cells in a lithium ion battery is a promising approach to reduce or mitigate these safety risks in a highly controllable manner.



#### COMMUNICATIONS

#### 2240

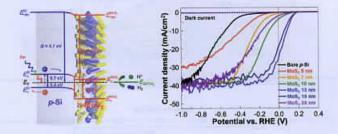
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# Wafer-scale transferable molybdenum disulfide thin-film catalysts for photoelectrochemical hydrogen production

Ki Chang Kwon, Seokhoon Choi, Kootak Hong, Cheon Woo Moon, Young-Seok Shim, Do Hong Kim, Taemin Kim, Woonbae Sohn, Jong-Myeong Jeon, Chul-Ho Lee, Ki Tae Nam, Seungwu Han, Soo Young Kim\* and Ho Won Jang\*

Wafer-scale n-MoS₂/p-Si photocathodes with high hydrogen evolution reaction activities are demonstrated.



#### 2249

# Dual coexisting interconnected graphene nanostructures for high performance supercapacitor applications

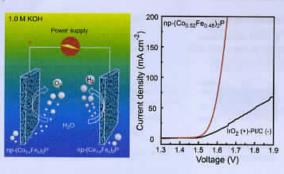
Hyun-Kyung Kim, Ali Reza Kamali,\* Kwang Chul Roh, Kwang-Bum Kim\* and Derek John Fray\*

A high-quality hierarchical carbon nanostructure consisting of graphene nanosheets and nanoscrolls can be synthesized by a facile and scalable molten salt method. This carbon nanostructure is here proposed as a high-performance supercapacitor electrode material.



#### COMMUNICATIONS

2257



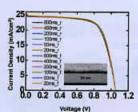
# Versatile nanoporous bimetallic phosphides towards electrochemical water splitting

Yongwen Tan, Hao Wang, Pan Liu, Yuhao Shen, Chun Cheng, Akihiko Hirata, Takeshi Fujita, Zheng Tang and Mingwei Chen\*

Nanoporous bimetallic (Co<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>P phosphides with tuneable Co/Fe ratios exhibit versatile catalytic activities for highly efficient electrochemical water splitting.

2262





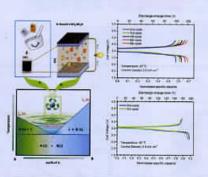


# Hysteresis-free low-temperature-processed planar perovskite solar cells with 19.1% efficiency

Heetae Yoon, Seong Min Kang, Jong-Kwon Lee\* and Mansoo Choi\* »

Hysteresis-free and highly efficient  $CH_3NH_3PbI_3$  perovskite solar cells employing a compact  $C_{60}$  material as an electron transport layer have been developed for the first time using both rigid glass and plastic substrates.

2267

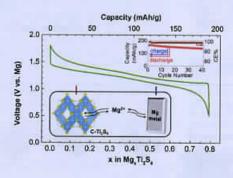


# A green and cost-effective rechargeable battery with high energy density based on a deep eutectic catholyte

Yarong Wang and Haoshen Zhou\*

Deep eutectic catholytes/anolytes, such as  $FeCl_3-6H_2O$ / urea, are potentially a class of low-cost and greener active electrolytes with high volumetric capacities.

2273



# A high capacity thiospinel cathode for Mg batteries

Xiaoqi Sun, Patrick Bonnick, Victor Duffort, Miao Liu, Ziqin Rong, Kristin A. Persson, Gerbrand Ceder and Linda F. Nazar\*

A Mg full cell with a thiospinel cathode material shows 190 mA h g<sup>-1</sup> capacity and relatively stable capacity retention.

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2278

### Light mar substrate optoelect

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Tian Li, Jia Doug Hen Liangbing We integral new type o optoelectro

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# Quantifica perovskite luminesce

Gilbert El-H Jorge Ávila, Michele Ses

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295

# Soft-cover perovskite solar cells

Fei Ye, Han Maoshu Yin Xudong Yar

A large area a high mater solution pro-

302

# Organic an by adhesive patterning

George D. S Michael Salv Peter Schwe Ning Li, Erdi Hans-Joach

We demonst fabrication re

### COMMUNICATIONS

#### 2275

# Light management in plastic-paper hybrid substrate towards high-performance optoelectronics

Yonggang Yao, Jinsong Tao, Jianhua Zou, Bilun Zhang, Tian Li, Jiaqi Dai, Mingwei Zhu, Sha Wang, Kun Kelvin Fu, Doug Henderson, Emily Hitz, Junbiao Peng\* and Liangbing Hu\*

We integrated plastic into mesoporous paper to achieve a new type of substrate plastic—paper for high performance optoelectronics.

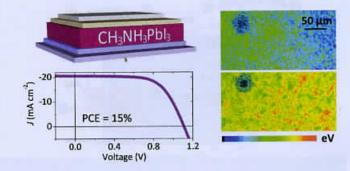


#### 2286

### Quantification of spatial inhomogeneity in perovskite solar cells by hyperspectral luminescence imaging

Gilbert El-Hajje, Cristina Momblona, Lidón Gil-Escrig, Jorge Ávila, Thomas Guillemot, Jean-François Guillemoles, Michele Sessolo, Henk J. Bolink\* and Laurent Lombez\*

Perovskite solar cells are analyzed by photo- and electroluminescence hyperspectral imaging. Significant spatial inhomogeneities in the quasi-Fermi level splitting are observed.

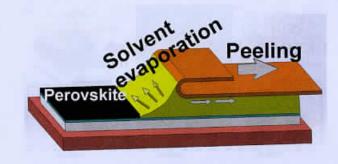


#### 2295

### Soft-cover deposition of scaling-up uniform perovskite thin films for high cost-performance solar cells

Fei Ye, Han Chen, Fengxian Xie, Wentao Tang, Maoshu Yin, Jinjin He, Enbing Bi, Yanbo Wang, Xudong Yang\* and Liyuan Han\*

A large area perovskite film with less structural defects and a high material utilization ratio was formed by a continuous solution processing method, soft-cover deposition.

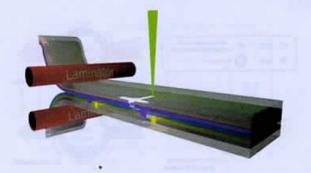


#### 2302

# Organic and perovskite solar modules innovated by adhesive top electrode and depth-resolved laser patterning

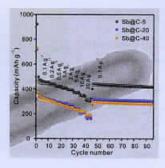
George D. Spyropoulos,\* César Omar Ramirez Quiroz, Michael Salvador, Yi Hou, Nicola Gasparini, Peter Schweizer, Jens Adams, Peter Kubis, Ning Li, Erdmann Spiecker, Tayebeh Ameri, Hans-Joachim Egelhaaf and Christoph J. Brabec

We demonstrate an innovative solution-processing fabrication route for organic and perovskite solar modules.



### COMMUNICATIONS

2314

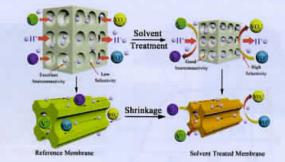


# Sb@C coaxial nanotubes as a superior long-life and high-rate anode for sodium ion batteries

Zhiming Liu, Xin-Yao Yu, Xiong Wen (David) Lou\* and Ungyu Paik\*

Sb@C coaxial nanotubes have been designed and synthesized using a facile strategy starting with  $Sb_2S_3$  nanorods. The as-obtained Sb@C nanotubes exhibit unprecedented sodium storage properties.

2319



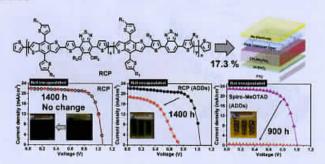
# High-performance porous uncharged membranes for vanadium flow battery applications created by tuning cohesive and swelling forces

Wenjing Lu, Zhizhang Yuan, Yuyue Zhao, Xianfeng Li,\* Huamin Zhang\* and Ivo F. J. Vankelecom

A simple and effective solvent treatment method was developed to prepare high-performance porous membranes with a tunable morphology for VFBs.

### PAPERS

2326

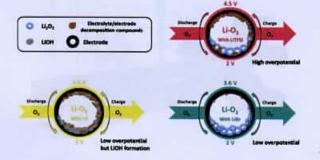


# Dopant-free polymeric hole transport materials for highly efficient and stable perovskite solar cells

Guan-Woo Kim, Gyeongho Kang, Jinseck Kim, Gang-Young Lee, Hong II Kim, Limok Pyeon, Jaechol Lee and Taiho Park\*

A dopant–free polymeric hole transport material (HTM), RCP, based on benzo[1,2-b:4,5:b']dithiophene and 2,1,3-benzothiadiazole exhibited a high efficiency of 17.3% in a perovskite solar cell and maintained its initial efficiency for over 1400 hours.

2334



# Li-O<sub>2</sub> cells with LiBr as an electrolyte and a redox mediator

Won-Jin Kwak, Daniel Hirshberg, Daniel Sharon, Michal Afri, Aryeh A. Frimer, Hun-Gi Jung, Doron Aurbach\* and Yang-Kook Sun\*

Improved efficiency and cyclability of cells containing LiBr demonstrate that the appropriate choice of electrolyte solution is the key to a successful Li-O<sub>2</sub> battery.

PAPERS

#### 2346

# precursors in neutral n

Carlo Santor Mounika Kor Orianna Brei Plamen Atan

Fe-based cat showed high AC (90-99%)

### 2354

# A comparat

Matthew R. S and Eric W. I

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Jeffery A. Ag Toshihiro Ad Joseph J. Be Kai Zhu\*

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# Pyroelectric tuning ther and magne

Gaurav Vats, Chris R. Bow Demonstratio

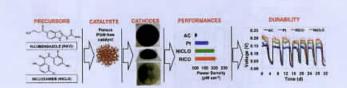
in ferroelectr nanostructur conversion e

#### 2346

# Iron based catalysts from novel low-cost organic precursors for enhanced oxygen reduction reaction in neutral media microbial fuel cells

Carlo Santoro, Alexey Serov, Lydia Stariha, Mounika Kodali, Jonathan Gordon, Sofia Babanova, Orianna Bretschger, Kateryna Artyushkova and Plamen Atanassov\*

Fe-based catalysts based on ricobendazole and niclosamide showed higher performance compared to Pt (20–25%) and AC (90–99%) and more durability in long terms operations.

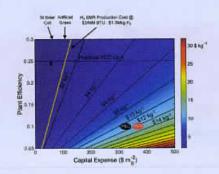


#### 2354

## A comparative technoeconomic analysis of renewable hydrogen production using solar energy

Matthew R. Shaner, Harry A. Atwater, Nathan S. Lewis\* and Eric W. McFarland\*

Solar H<sub>2</sub> production cost (\$ kg<sup>-1</sup>) techno-economic landscape for photoelectrochemical (PEC) and photovoltaic-electrolysis (PV-E). References include conventional H<sub>2</sub> production, robust outdoor material (artificial grass) and solar cell.

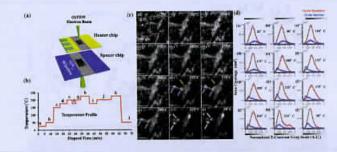


#### 2372

# In situ investigation of the formation and metastability of formamidinium lead tri-iodide perovskite solar cells

Jeffery A. Aguiar,\* Sarah Wozny, Terry G. Holesinger, Toshihiro Aoki, Maulik K. Patel, Mengjin Yang, Joseph J. Berry, Mowafak Al-Jassim, Weilie Zhou\* and Kai Zhu\*

Organic-inorganic perovskites have emerged as an important class of next generation solar cells due to their remarkable low cost, band gap, and sub-900 nm absorption onset.

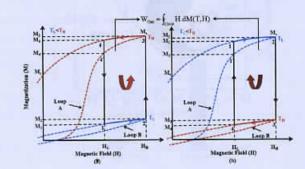


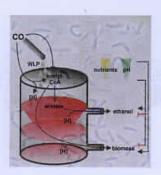
#### 2383

# Pyroelectric control of magnetization for tuning thermomagnetic energy conversion and magnetocaloric effect

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

Demonstration of pyroelectric control of magnetization in ferroelectric/magnetic/ferroelectric multi-layered nanostructures for tuning thermomagnetic energy conversion efficiency and magnetocaloric effect.





# Ethanol production in syngas-fermenting Clostridium ljungdahlii is controlled by thermodynamics rather than by enzyme expression

H. Richter, B. Molitor, H. Wei, W. Chen, L. Aristilde\* and L. T. Angenent\*

A simplified overflow model (depicted as a rain barrel) is proposed to explain how ethanol is produced during syngas fermentation.

2400

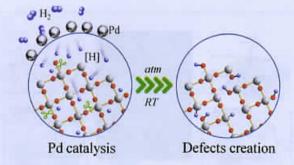


# First demonstration of direct hydrocarbon fuel production from water and carbon dioxide by solar-driven thermochemical cycles using rhodium-ceria

Fangjian Lin, Matthäus Rothensteiner, Ivo Alxneit,\* Jeroen A. van Bokhoven and Alexander Wokaun

Sustained production of methane directly from water and carbon dioxide by solar-driven thermochemical cycles is achieved for the first time with rhodium on ceria.

2410

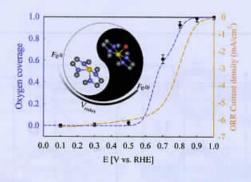


# Pd-catalyzed instant hydrogenation of TiO<sub>2</sub> with enhanced photocatalytic performance

Yingfeng Xu, Chen Zhang, Lingxia Zhang, Xiaohua Zhang, Heliang Yao and Jianlin Shi\*

This facile hydrogenation strategy is based on room temperature H2 dissociation into [H] on Pd, providing a general methodology for transitional metal oxide hydrogenation under ordinary conditions for advanced photocatalysis systems.

2418



# Structural and mechanistic basis for the high activity of Fe-N-C catalysts toward oxygen reduction

Jingkun Li, Shraboni Ghoshal, Wentao Liang, Moulay-Tahar Sougrati, Frédéric Jaouen, Barr Halevi, Samuel McKinney, Geoff McCool, Chunrong Ma, Xianxia Yuan, Zi-Feng Ma, Sanjeev Mukerjee\* and Qingying Jia\*

The biomimetic dynamic nature of the Fe-N-C active site with a near-optimal  $Fe^{2+/3+}$  redox potential facilitates ORR by balancing the site-blocking effect and O2 dissociation.

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Linchao Mu Zhiliang Wa Ruotian Chi Can Li\*

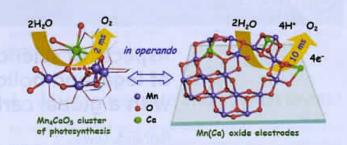
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#### ONEX

Water oxidation catalysis – role of redox and structural dynamics in biological photosynthesis and inorganic manganese oxides

I. Zaharieva,\* D. González-Flores, B. Asfari, C. Pasquini, M. R. Mohammadi, K. Klingan, I. Zizak, S. Loos, P. Chernev and H. Dau\*

Water oxidation is pivotal in biological photosynthesis, where it is catalyzed by a protein-bound metal complex with a Mn<sub>4</sub>Ca-oxide core; related synthetic catalysts may become key components in non-fossil fuel technologies.



#### 2444

Elimination of the light soaking effect and performance enhancement in perovskite solar cells using a fullerene derivative

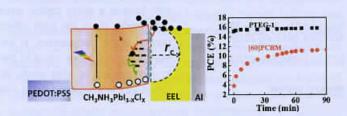
S. Shao, M. Abdu-Aguye, L. Qiu, L.-H. Lai, J. Liu,

S. Adjokatse, F. Jahani, M. E. Kamminga,

G. H. ten Brink, T. T. M. Palstra, B. J. Kooi,

J. C. Hummelen and M. Antonietta Loi\*

The higher dielectric constant and electron donating properties of PTEG-1 electron extraction layer synergistically helps to eliminate the light soaking effect and enhance device performance.

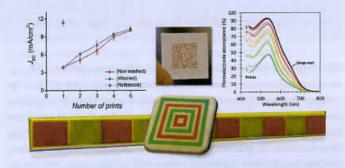


#### 2453

### Dye-sensitized solar cells with inkjet-printed dyes

Syed Ghufran Hashmi, Merve Özkan, Janne Halme,\* Shaik Mohammed Zakeeruddin, Jouni Paltakari, Michael Grätzel and Peter D. Lund

Inkjet printing dyes on TiO<sub>2</sub> films enables the creation of DSSCs with tailored transparency, color density gradients, and patterns of multiple dyes on the same photoelectrode.



#### 2463

Enhancing charge separation on high symmetry SrTiO<sub>3</sub> exposed with anisotropic facets for photocatalytic water splitting

Linchao Mu, Yue Zhao, Ailong Li, Shengyang Wang, Zhiliang Wang, Jingxiu Yang, Yi Wang, Taifeng Liu, Ruotian Chen, Jian Zhu, Fengtao Fan, Rengui Li\* and Can Li\*

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Spatial charge separation achieved on the anisotropic facets of high symmetry  $SrTiO_3$  nanocrystals for highly efficient photocatalytic overall water splitting.

