## **Energy & Environmental Science**

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### IN THIS ISSUE

ISSN 1754-5692 CODEN EESNBY 9(1) 1-268 (2016)



## Cover

See Félix Urbain et al., pp. 145-154. Image reproduced by permission of Félix Urbain from Energy Environ. Sci., 2016, 9, 145.



### Inside cover

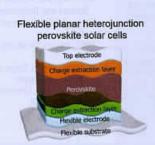
See Tae-Woo Lee et al., pp. 12-30. Image reproduced by permission of Tae-Woo Lee from Energy Environ. Sci., 2016, 9, 12.

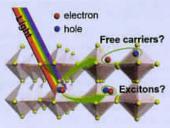
### REVIEWS

### Planar heterojunction organometal halide perovskite solar cells: roles of interfacial layers

Hobeom Kim, Kyung-Geun Lim and Tae-Woo Lee\*

This review article gives an overview of progress in planar heterojunction perovskite solar cells and the roles of interfacial layers in the device, and suggests a practical strategy to fabricate highly efficient and flexible planar heterojunction perovskite solar cells.

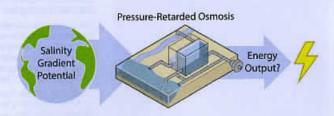


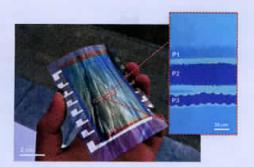


### Pressure-retarded osmosis for power generation from salinity gradients: is it viable?

Anthony P. Straub, Akshay Deshmukh and Menachem Elimelech\*

We review pressure-retarded osmosis focusing on the net energy extractable from the process and the ultimate viability of various configurations.





Highly efficient, large area, roll coated flexible and rigid OPV modules with geometric fill factors up to 98.5% processed with commercially available Claudiu B. Buc

L. Lucera,\* F. Machui, P. Kubis, H. D. Schmidt, J. Adams, S. Strohm, T. Ahmad, K. Forberich, H.-J. Egelhaaf\* and C. J. Brabec

Flexible roll-coated and rigid organic PV modules, solution processed on a large area, are reported with efficiencies of 4.2% and 5.3%, respectively.

A soft, multila

John Muldoon

It is desirable th flexible and self expansion durir impede electro

Superior performance of borocarbonitrides, B<sub>x</sub>C<sub>v</sub>N<sub>z</sub>, as stable, low-cost metal-free electrocatalysts for the hydrogen evolution reaction

Manjeet Chhetri, Somak Maitra, Himanshu Chakraborty, Umesh V. Waghmare and C. N. R. Rao\*

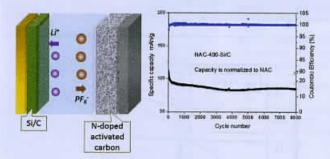
We report superior hydrogen evolution activity of metal-free borocarbonitride (BCN) catalysts.

Energy savin bistable low-

Haijin Shin, Se Minsu Han an

Energy saving controlling the level (EHOMO " bistable electr electrolyte lay at the voltage (879 cm2 C

102



Nitrogen-doped activated carbon for a high energy hybrid supercapacitor

Bing Li, Fang Dai, Qiangfeng Xiao, Li Yang, Jingmei Shen, Cunman Zhang\* and Mei Cai\*

The present work provides a novel one-step synthesis for nitrogen-doped activated carbon. The excellent performance of the N-doped AC allows its further application in a hybrid-type supercapacitor, which utilizes a combination of the capacitor electrode and a Li-ion battery anode.

Single layer metals as hi water oxida

Xiaoju Cui, P Xinhe Bao\*

Single layer g 3d transition and durability



Metal-organic-framework-engaged formation of Co nanoparticle-embedded carbon@Co<sub>9</sub>S<sub>8</sub> double-shelled nanocages for efficient oxygen reduction

Han Hu, Lei Han, Mengzhou Yu, Zhiyu Wang\* and Xiong Wen (David) Lou\*

Rationally designed Co nanoparticle-embedded carbon@Co<sub>9</sub>S<sub>8</sub> double-shelled nanocages exhibit excellent electrocatalytic performance for the oxygen reduction reaction.

Molecular-Culn(S,Se)<sub>2</sub> solar cells

A. R. Uhl,\* J

Metal-organ oxidation sta composition

### COMMUNICATIONS

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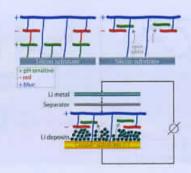
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nen,

### A soft, multilayered lithium-electrolyte interface

Claudiu B. Bucur, Adrian Lita, Naoki Osada and John Muldoon\*

It is desirable that a thin film lithium—electrolyte interface is flexible and self-healing to accommodate the large volume expansion during lithium deposition without rupturing and impede electrolyte decomposition.

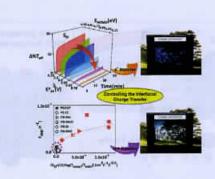


### 117

### Energy saving electrochromic windows from bistable low-HOMO level conjugated polymers

Haijin Shin, Seogjae Seo, Chihyun Park, Jongbeom Na, Minsu Han and Eunkyoung Kim\*

Energy saving electrochromic windows were achieved by controlling the interfacial charge transfer using low-HOMO level ( $E_{\text{HOMO}} < -5 \text{ eV}$ )  $\pi$ -conjugated polymers (CPs) as bistable electrochromic films and an ionic liquid as the electrolyte layer. It provided a long bistability (>90 min) at the voltage-off state with a high coloration efficiency (879 cm² C $^{-1}$ ).

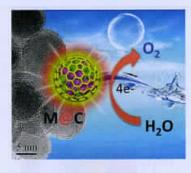


### 123

## Single layer graphene encapsulating non-precious metals as high-performance electrocatalysts for water oxidation

Xiaoju Cui, Pengju Ren, Dehui Deng,\* Jiao Deng and Xinhe Bao\*

Single layer graphene encapsulating earth-abundant 3d transition metal nanoparticles exhibits excellent activity and durability for water oxidation, even exceeding IrO<sub>2</sub>.



### 130

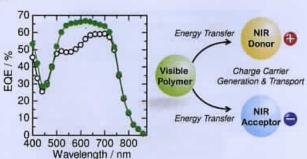
# Molecular-ink route to 13.0% efficient low-bandgap Culn(S,Se)<sub>2</sub> and 14.7% efficient Cu(In,Ga)(S,Se)<sub>2</sub> solar cells

A. R. Uhl, \* J. K. Katahara and H. W. Hillhouse \*

Metal-organic complexes were found critical to control oxidation states, loss of metals during processing, and the composition of the absorber.



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High-performance ternary blend all-polymer solar cells with complementary absorption bands from visible to near-infrared wavelengths

Hiroaki Benten,\* Takaya Nishida, Daisuke Mori, Huajun Xu, Hideo Ohkita and Shinzaburo Ito\*

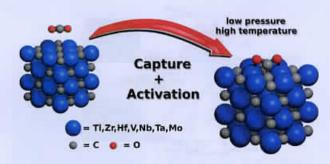
Ternary blend all-polymer solar cells open a new avenue for accelerating improvement in the efficiency of non-fullerene thin-film organic photovoltaics. 164

### A scanning of surface n photocatho

Jesus M. Vel Adam Pieteri Zhuangqun I Bruce S. Bru

Microscale in performance photocathod microscopy.

141



### Transition metal carbides as novel materials for CO<sub>2</sub> capture, storage, and activation

Christian Kunkel, Francesc Viñes and Francesc Illas\*

Transition metal carbides are posed as promising materials for carbon dioxide (CO<sub>2</sub>) capture and storage at room temperature and low pressures, as shown by density functional simulations on proper models, and estimates of adsorption/desorption rates. Aside, the activated nature of the adsorbed CO<sub>2</sub> opens the path for its conversion into other valuable chemicals.

176

### Optimizing

Jae-II Jung, Gyutae Nam Jaephil Cho

oxygen ele

The success electrocataly of energy stepresented.

**PAPERS** 

145



# Multijunction Si photocathodes with tunable photovoltages from 2.0 V to 2.8 V for light induced water splitting

Félix Urbain,\* Vladimir Smirnov, Jan-Philipp Becker, Andreas Lambertz, Florent Yang, Jürgen Ziegler, Bernhard Kaiser, Wolfram Jaegermann, Uwe Rau and Friedhelm Finger

Bias-free solar water splitting is demonstrated using thin film silicon based triple and quadruple junction solar cells with solar-to-hydrogen efficiencies up to 9.5%.

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Structural water oxid forms of li

Graeme Ga Yong Bok G G. Charles

Comparisor LiCoO<sub>2</sub> sho LiCo<sub>2</sub>O<sub>4</sub> spi performance

103

## Design of for production CO<sub>2</sub>

Meenesh F

The design is proposed natural pho

tetragonal cubic

Structural and optical properties of methylammonium lead iodide across the tetragonal to cubic phase transition: implications for perovskite solar cells

Claudio Quarti,\* Edoardo Mosconi, James M. Ball, Valerio D'Innocenzo, Chen Tao, Sandeep Pathak, Henry J. Snaith, Annamaria Petrozza\* and Filippo De Angelis\*

We report optical measurements on MAPbl<sub>3</sub> solar cells, together with *ab initio* simulations, to investigate the material property changes across the tetragonal to cubic phase transition.

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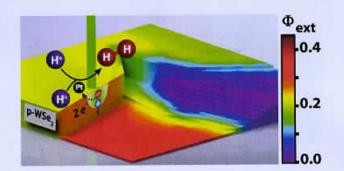
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# A scanning probe investigation of the role of surface motifs in the behavior of p-WSe<sub>2</sub> photocathodes

Jesus M. Velazquez, Jimmy John, Daniel V. Esposito, Adam Pieterick, Ragip Pala, Guofeng Sun, Xinghao Zhou, Zhuangqun Huang, Shane Ardo, Manuel P. Soriaga, Bruce S. Brunschwig and Nathan S. Lewis\*

Microscale in situ interrogation of the photoelectrochemical performance of pristine and Pt-covered p-WSe<sub>2</sub> photocathodes was studied by scanning photocurrent microscopy.

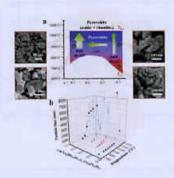


176

### Optimizing nanoparticle perovskite for bifunctional oxygen electrocatalysis

Jae-Il Jung, Marcel Risch, Seungkyu Park, Min Gyu Kim, Gyutae Nam, Hu-Young Jeong, Yang Shao-Horn\* and Jaephil Cho\*

The successful synthesis of bifunctional perovskite electrocatalysts  $\sim$  50 nm in size towards the development of energy storage systems with high power density is presented.

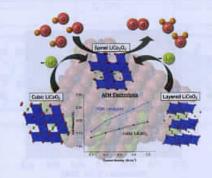


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### Structural basis for differing electrocatalytic water oxidation by the cubic, layered and spinel forms of lithium cobalt oxides

Graeme Gardner, Jafar Al-Sharab, Nemanja Danilovic, Yong Bok Go, Katherine Ayers, Martha Greenblatt and G. Charles Dismukes\*

Comparison of the OER activity of cubic and layered LiCoO<sub>2</sub> shows a convergence to the catalytically active LiCo<sub>2</sub>O<sub>4</sub> spinel phase, which demonstrates excellent performance in membrane-based alkaline electrolysis.



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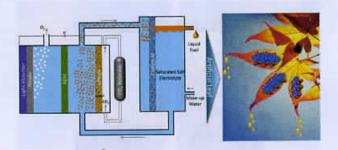
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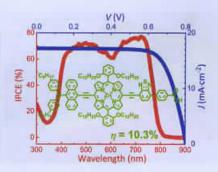
2016

### Design of an artificial photosynthetic system for production of alcohols in high concentration from CO<sub>2</sub>

Meenesh R. Singh and Alexis T. Bell\*

The design for a novel artificial photosynthetic system is proposed that can be ten-fold more efficient than natural photosynthesis and produce almost pure liquid fuel.





### Porphyrins bearing a consolidated anthryl donor with dual functions for efficient dye-sensitized solar cells

Chin-Li Wang, Min Zhang, Yu-Hsin Hsiao, Chuan-Kai Tseng, Chia-Lin Liu, Mingfei Xu, Peng Wang\* and Ching-Yao Lin\*

Novel layered solid oxide fuel cells with multiple-twinned Ni<sub>0.8</sub>Co<sub>0.2</sub> nanoparticles:

Bin Hua, Ning Yan, Meng Li, Ya-qian Zhang, Yi-fei Sun,

Jian Li, Thomas Etsell, Partha Sarkar, Karl Chuang and

To energy-efficiently offset our carbon footprint, we

developed a layered H-SOFC with multiple-twinned Ni<sub>0.8</sub>Co<sub>0.2</sub> nanoparticles, achieving three milestones: CO<sub>2</sub> utilization, electricity generation and syngas production.

Polyethylenimine promoted electrocatalytic reduction of CO<sub>2</sub> to CO in aqueous medium

by graphene-supported amorphous molybdenum

Fengwang Li, Shu-Feng Zhao, Lu Chen, Azam Khan,

polyethylenimine modified reduced graphene oxide can

catalyse the electroreduction of CO2 to CO or "syngas"

Amorphous molybdenum sulphide immobilized on

Douglas R. MacFarlane\* and Jie Zhang\*

in aqueous media with high efficiency.

and power-chemical cogeneration

Jing-Li Luo\*

sulphide

Efficient DSSC performance was achieved by using a porphyrin dye bearing a consolidated anthryl donor which provides both electron-donating and absorption-broadening effects.

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the key to thermally independent CO2 utilization

using a wetself-organize PTB7 and PC maximum ef

Michael D.



PP13TFSI

0.0

CO.+H,O

-0.6 -0.4 -0.2 Potential / V vs. RHE

### To mitigate self-discharge of lithium-sulfur batteries by optimizing ionic liquid electrolytes

Lina Wang, Jingyuan Liu, Shouyi Yuan, Yonggang Wang\* and Yongyao Xia\*

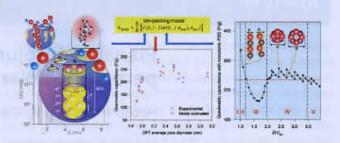
Here we demonstrate pronounced suppression of selfdischarge using an ionic liquid of N-methyl-N-propylpiperidinium bis(trifluoromethanesulfonyl)imide-based electrolytes for Li-S batteries.

### 232

# Geometrically confined favourable ion packing for high gravimetric capacitance in carbon-ionic liquid supercapacitors

Xuehang Wang, Haitao Zhou, Edel Sheridan, John Charles Walmsley, Dingding Ren and De Chen\*

The specific energy of carbon-ionic liquid supercapacitors comparable to NiMH batteries has been achieved by a combined modeling and experimental approach.

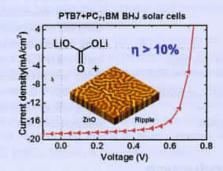


### 240

## Highly efficient inverted bulk-heterojunction solar cells with a gradiently-doped ZnO layer

Sungho Nho, Gyoelim Baek, Sujung Park, Bo Ram Lee, Myung Joo Cha, Dong Chan Lim, Jung Hwa Seo, Seung-Hwan Oh, Myoung Hoon Song and Shinuk Cho\*

Highly efficient inverted BHJ solar cells were demonstrated using a wet-chemically prepared doped ZnO layer with a self-organized ripple nanostructure. The solar cell based on PTB7 and  $PC_{71}BM$  with  $Ll_2CO_3$ -doped ZnO layer yielded a maximum efficiency of 10.08%.

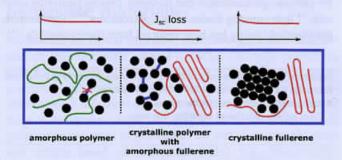


### 247

# Morphological and electrical control of fullerene dimerization determines organic photovoltaic stability

Thomas Heumueller, William R. Mateker, Andreas Distler, Urs F. Fritze, Rongrong Cheacharoen, William H. Nguyen, Markus Biele, Michael Salvador, Max von Delius, Hans-Joachim Egelhaaf, Michael D. McGehee\* and Christoph J. Brabec\*

Light induced fullerene dimerization is controlled by both the fullerene and polymer morphology of organic solar cells.



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## Open circuit voltage and efficiency in ternary organic photovoltaic blends

N. Felekidis, E. Wang\* and M. Kemerink\*

We develop the understanding of the open circuit voltage and efficiency in ternary organic solar cells through experiments and quantitative modeling.

