

## IN THIS ISSUE

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**Cover**  
See Lou, Aydil *et al.*,  
pp. 2592–2597.  
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**Inside cover**  
See Galli *et al.*,  
pp. 2598–2602.  
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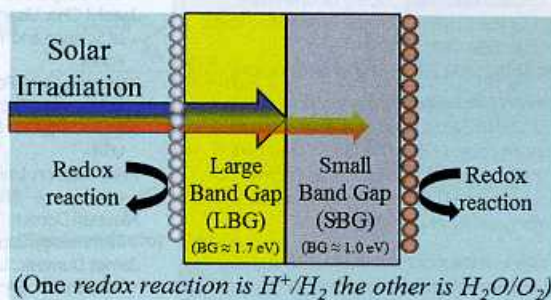
## ANALYSIS

2397

### 2-Photon tandem device for water splitting: comparing photocathode first versus photoanode first designs

Brian Seger, Ivano E. Castelli, Peter C. K. Vesborg,  
Karsten W. Jacobsen, Ole Hansen and Ib Chorkendorff\*

This work analyzes the differences between a 'photoanode first' and a 'photocathode first' 2-photon water splitting device.



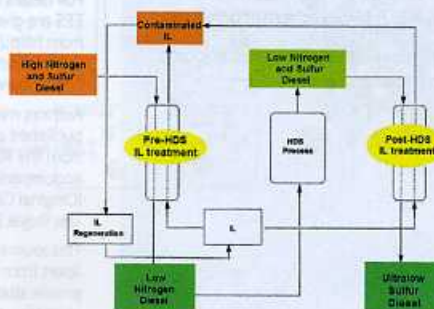
## REVIEWS

2414

### Applications of ionic liquids in the removal of contaminants from refinery feedstocks: an industrial perspective

Rafael Martínez-Palou\* and Rafael Luque

Ionic liquids are novel, green and efficient compounds for the removal of contaminants from refinery feedstocks.



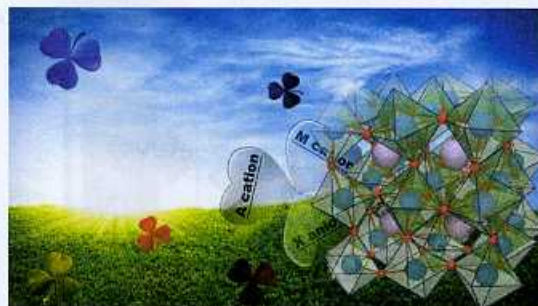


2448

### Organohalide lead perovskites for photovoltaic applications

Peng Gao,\* Michael Grätzel  
and Mohammad K. Nazeeruddin\*

This review presents the state-of-the-art organohalide lead perovskites, which are currently making an immense impact across the photovoltaic community.

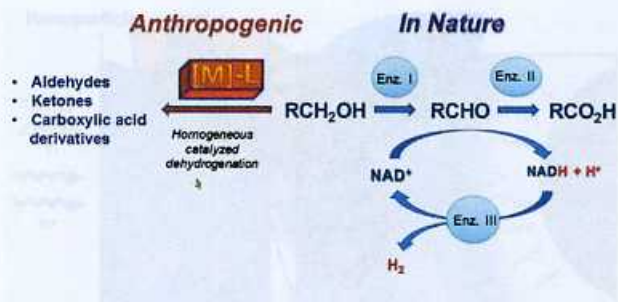


2464

### Molecular catalysts for hydrogen production from alcohols

Monica Trincado, Dipshikha Banerjee  
and Hansjörg Grützmacher

The conversion of alcohols to carbonyl compounds and hydrogen: a survey of homogeneous enzymatic and anthropogenic catalytic dehydrogenation reactions.

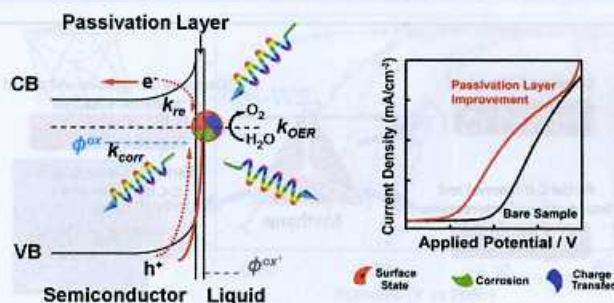


2504

### Enhanced photoelectrochemical water-splitting performance of semiconductors by surface passivation layers

Rui Liu, Zhi Zheng, Joshua Spurgeon and Xiaogang Yang\*

This review paper summarized recent studies on improving the efficiency of semiconductor-based solar water-splitting devices by introducing surface passivation layers.

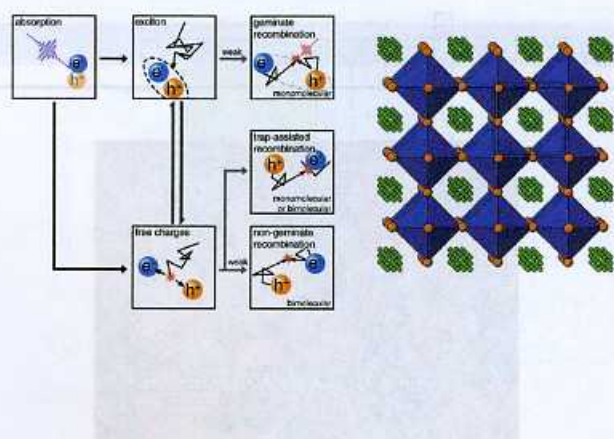


2518

### Advancements in perovskite solar cells: photophysics behind the photovoltaics

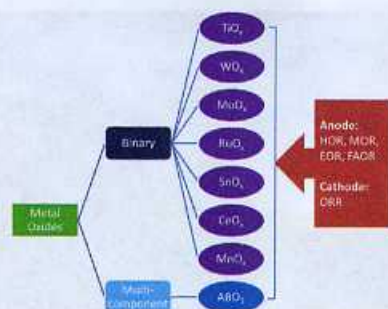
Tze Chien Sum\* and Nripan Mathews\*

This article reviews the fundamental photophysics and working mechanisms of perovskite solar cells and highlights the current state-of-the-art and open questions in this maturing field.





2535



### An overview of metal oxide materials as electrocatalysts and supports for polymer electrolyte fuel cells

Zhonghua Zhang,\* Jie Liu, Junjie Gu, Liang Su and Lifeng Cheng

In this review, we discuss the use of binary and multi-component metal oxides as independent electrocatalysts, co-catalysts and supports for various anode oxidation and cathode reduction reactions in polymer electrolyte fuel cells.

2559



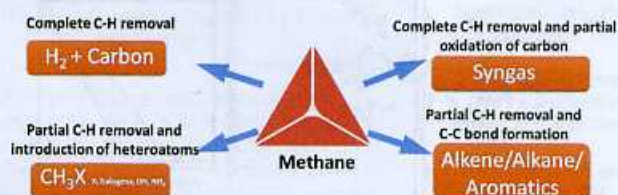
### Construction of one-dimensional nanostructures on graphene for efficient energy conversion and storage

Jia Le Xie, Chun Xian Guo and Chang Ming Li\*

This review summarizes the recent development of one-dimensional nanostructures constructed on graphene as electrodes have unique physico-chemical properties to synergistically offer highly-efficient energy conversion and storage.

## MINIREVIEW

2580



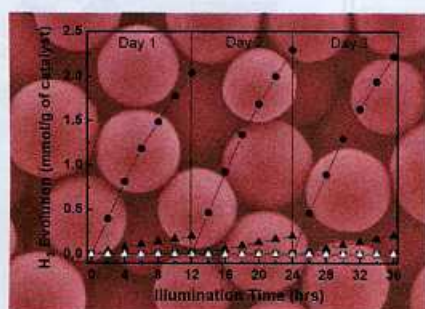
### Methane activation: the past and future

Pei Tang, Qingjun Zhu, Zhaoxuan Wu and Ding Ma\*

This review summarizes and provides an outlook on the possible routes for methane conversion to valuable fuel and chemicals.

## COMMUNICATIONS

2592



### Doping high-surface-area mesoporous TiO<sub>2</sub> microspheres with carbonate for visible light hydrogen production

Bin Liu, Li-Min Liu, Xiu-Feng Lang, Hsin-Yi Wang, Xiong Wen (David) Lou\* and Eray S. Aydil\*

Carbonate-doped mesoporous TiO<sub>2</sub> microspheres exhibit very high photocatalytic activity for visible light hydrogen production and degradation of methyl orange.

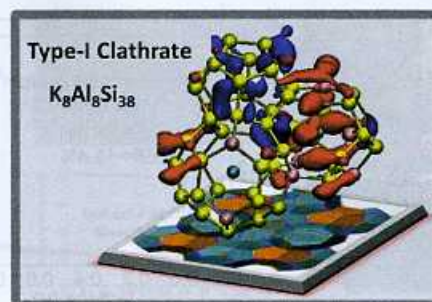


2598

### Si-based Earth abundant clathrates for solar energy conversion

Yuping He, Fan Sui, Susan M. Kauzlarich and Giulia Galli\*

We synthesized a Si-based clathrate, composed entirely of Earth abundant elements, and using *ab initio* calculations and spectroscopic and Hall mobility measurement showed that it is a promising material for solar energy conversion.

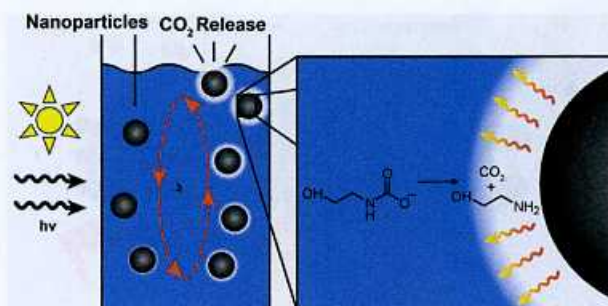


2603

### Photothermal release of $CO_2$ from capture solutions using nanoparticles

Du T. Nguyen, Richard Truong, Richard Lee, Samantha A. Goetz and Aaron P. Esser-Kahn\*

We report the use of actinic light for the photo-thermal enhanced regeneration of  $CO_2$  from capture solutions containing nanoparticles. Regeneration efficiency increased with higher nanoparticle concentrations and initial solution temperatures.

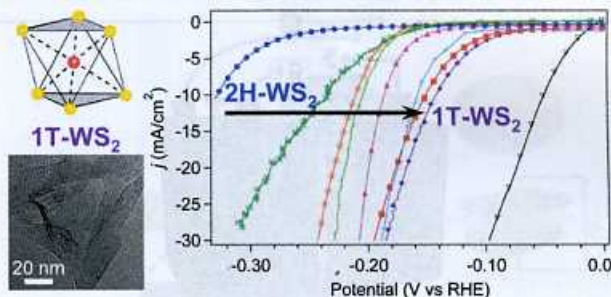


2608

### Highly active hydrogen evolution catalysis from metallic $WS_2$ nanosheets

Mark A. Lukowski, Andrew S. Daniel, Caroline R. English, Fei Meng, Audrey Forticaux, Robert J. Hamers and Song Jin\*

Metallic  $WS_2$  nanosheets chemically exfoliated from chemical vapour deposited  $WS_2$  nanostructures display excellent catalytic activity for the hydrogen evolution reaction.

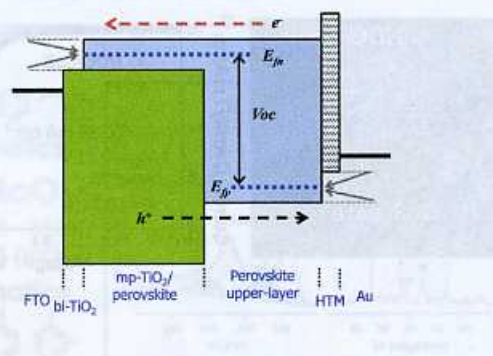


2614

### Voltage output of efficient perovskite solar cells with high open-circuit voltage and fill factor

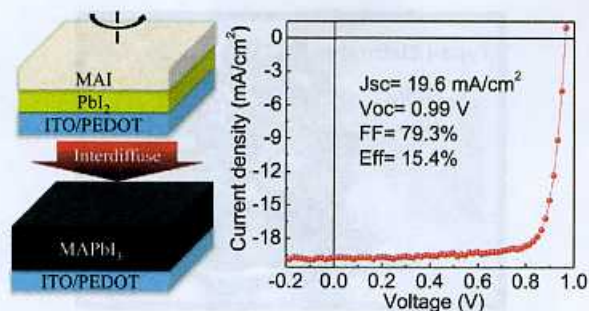
Seungchan Ryu, Jun Hong Noh, Nam Joong Jeon, Young Chan Kim, Woon Seok Yang, Jangwon Seo and Sang Il Seok\*

The voltage output of perovskite solar cells is found to be dependent on both the energy level of perovskite itself as a solar absorber and hole transporting materials.





2619

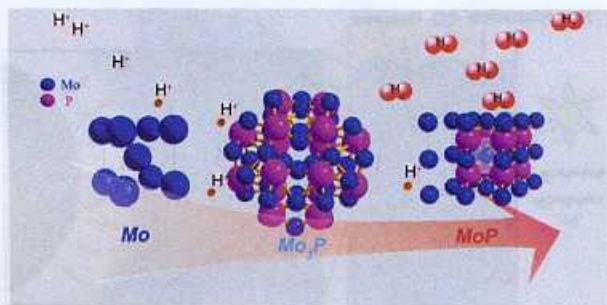


### Efficient, high yield perovskite photovoltaic devices grown by interdiffusion of solution-processed precursor stacking layers

Zhengguo Xiao, Cheng Bi, Yuchuan Shao, Qingfeng Dong, Qi Wang, Yongbo Yuan, Chenggong Wang, Yongli Gao and Jinsong Huang\*

A new low-temperature all-solution approach was invented to produce perovskite solar cells with an efficiency of 15.4% at high device yield.

2624

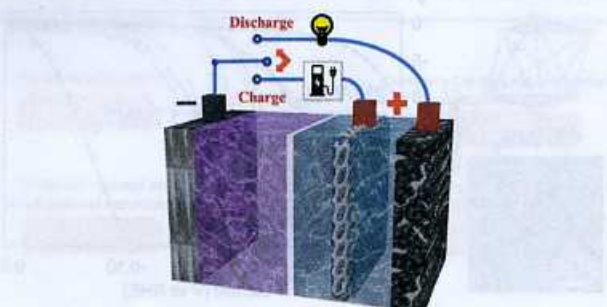


### Molybdenum phosphide as an efficient electrocatalyst for the hydrogen evolution reaction

Peng Xiao, Mahasin Alam Sk, Larissa Thia, Xiaoming Ge, Rern Jern Lim, Jing-Yuan Wang, Kok Hwa Lim and Xin Wang\*

The phosphorization of molybdenum leads to a good non-noble metal catalyst for the hydrogen evolution reaction in both acidic and alkaline conditions.

2630

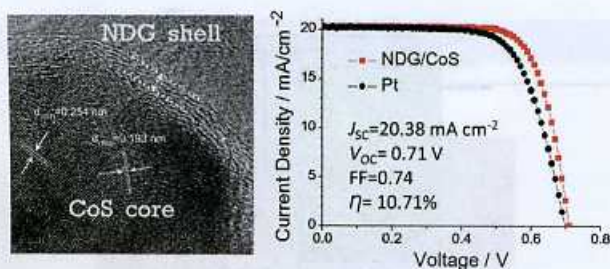


### Advanced hybrid Li-air batteries with high-performance mesoporous nanocatalysts

Longjun Li, Song-Hai Chai, Sheng Dai and Arumugam Manthiram\*

Advanced hybrid Li-air batteries are enabled by decoupled, high-performance mesoporous nanocatalysts.

2637



### A quasi core-shell nitrogen-doped graphene/cobalt sulfide conductive catalyst for highly efficient dye-sensitized solar cells

Enbing Bi, Han Chen,\* Xudong Yang, Wenqin Peng, Michael Grätzel and Liyuan Han\*

A platinum-free counter electrode was designed based on a quasi core-shell N-doped graphene/cobalt sulfide with high catalytic activity and conductivity.

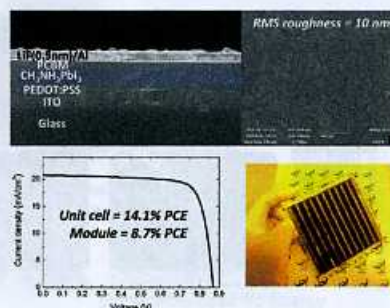


2642

### Benefits of very thin PCBM and LiF layers for solution-processed p-i-n perovskite solar cells

Jangwon Seo, Sangman Park, Young Chan Kim, Nam Joong Jeon, Jun Hong Noh, Sung Cheol Yoon\* and Sang Il Seok\*

Optimal thickness of a PCBM layer and insertion of the LiF interlayer on a well-controlled flat surface of the perovskite film are essential for fabricating planar perovskite-PCBM solar cells.

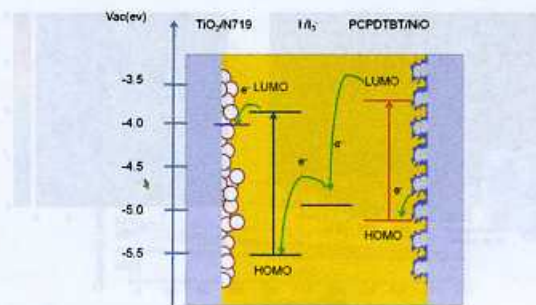


2647

### Polymer based photocathodes for panchromatic tandem dye-sensitized solar cells

ZhiPeng Shao, Xu Pan,\* HaiWei Chen, Li Tao, WenJun Wang, Yong Ding, Bin Pan, Shangfeng Yang and Songyuan Dai\*

A novel polymer based photocathode with a secondary porous structure was developed for tandem dye-sensitized solar cells (pn-DSCs). Complementary absorption was realized in pn-DSCs. The resulting tandem devices achieved a panchromatic absorption and a power conversion efficiency of 1.30%.



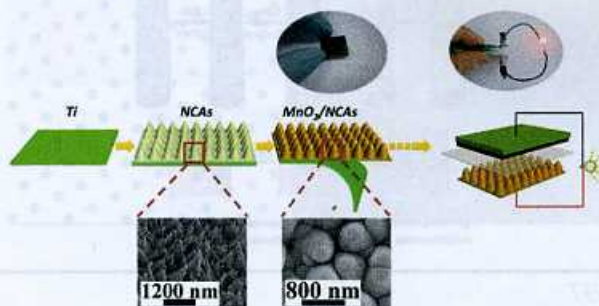
## PAPERS

2652

### Scalable fabrication of MnO<sub>2</sub> nanostructure deposited on free-standing Ni nanocone arrays for ultrathin, flexible, high-performance micro-supercapacitor

Zijin Su, Cheng Yang,\* Binghe Xie, Ziyin Lin, Zhexu Zhang, Jingping Liu, Baohua Li, Feiyu Kang and Ching Ping Wong

A thin film of Ni nanocone arrays loaded with MnO<sub>2</sub> nanostructures is prepared by an electro-deposition process and peeled off from the carrier substrate. This electrode shows superior performance for micro-supercapacitors.

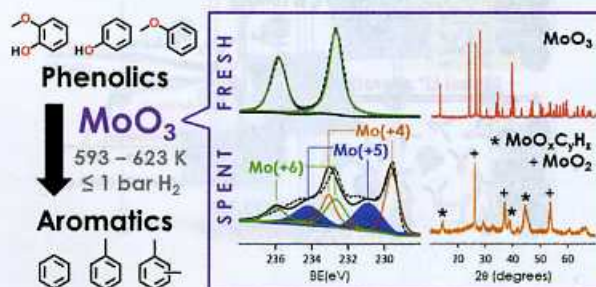


2660

### Insights into the catalytic activity and surface modification of MoO<sub>3</sub> during the hydrodeoxygenation of lignin-derived model compounds into aromatic hydrocarbons under low hydrogen pressures

Teerawit Prasomsri, Manish Shetty, Karthick Murugappan and Yuriy Román-Leshkov\*

MoO<sub>3</sub> is an effective catalyst for the hydrodeoxygenation (HDO) of lignin-derived oxygenates to generate high yields of aromatic hydrocarbons without ring-saturated products.





2670

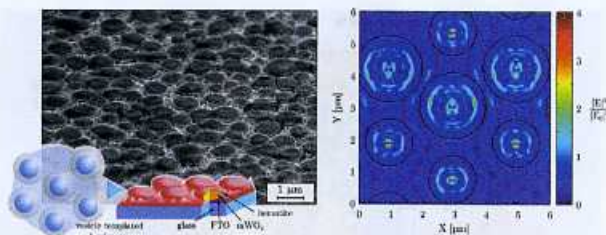


### Evolution of disposable bamboo chopsticks into uniform carbon fibers: a smart strategy to fabricate sustainable anodes for Li-ion batteries

Jian Jiang, Jianhui Zhu, Wei Ai, Zhanxi Fan, Xiaonan Shen, Chenji Zou, Jinping Liu, Hua Zhang and Ting Yu\*

Uniform carbon fibers evolved from bamboo chopsticks garbage are achieved by a facile hydrothermal method, exhibiting competitive electrochemical behavior with commercial graphite, or pretty high anodic performance after being optimized.

2680

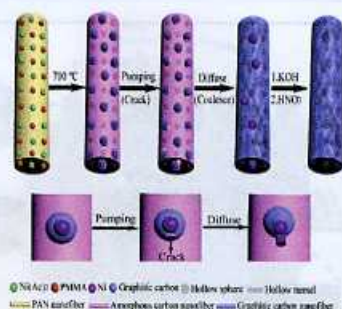


### Photonic light trapping in self-organized all-oxide microspheroids impacts photoelectrochemical water splitting

Florent Boudoire,\* Rita Toth, Jakob Heier, Artur Braun and Edwin C. Constable

A SEM picture of the microspheroids (tilted), scheme depicting the vesicle templated sol-gel process and squared normalized electric field intensity distribution inside the microspheroid calculated by finite-difference time-domain simulation.

2689

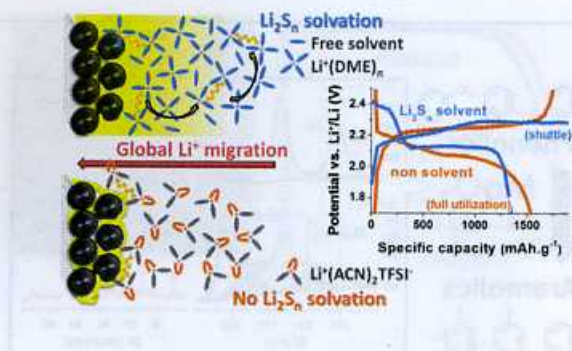


### Hollow-tunneled graphitic carbon nanofibers through Ni-diffusion-induced graphitization as high-performance anode materials

Yuming Chen, Xiaoyan Li, Xiangyang Zhou,\* Haimin Yao, Haitao Huang, Yiu-Wing Mai and Limin Zhou\*

Activated N-doped hollow-tunneled graphitic carbon nanofibers with a novel architecture are excellent anode materials for lithium ion batteries, displaying a superhigh reversible specific capacity and a remarkable volumetric capacity with outstanding rate capability and good cycling stability.

2697



### Unique behaviour of nonsolvents for polysulphides in lithium-sulphur batteries

M. Cuisinier, P.-E. Cabelguen, B. D. Adams, A. Garsuch, M. Balasubramanian and L. F. Nazar\*

Combination of a solvent-salt complex [acetonitrile(ACN)<sub>2</sub>-LiTFSI] with a hydrofluoroether (HFE) co-solvent unveils a new class of Li-S battery electrolytes that possess essentially no solubility for lithium polysulfides, yet exhibit excellent capacity and very good rate capability.

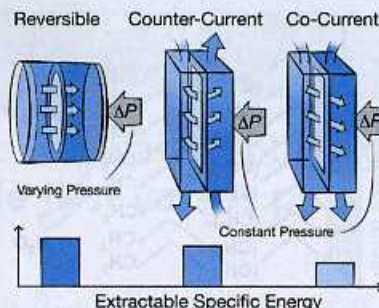


2706

### Thermodynamic limits of extractable energy by pressure retarded osmosis

Shihong Lin, Anthony P. Straub and Menachem Elimelech\*

The maximum specific energy obtainable in pressure retarded osmosis and the corresponding optimal operating conditions are analytically determined for three different operation modes: an ideal reversible process, and constant-pressure systems with either co-current flow or counter-current flow in a membrane module.

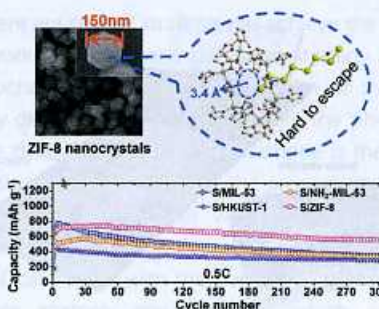


2715

### Rational design of a metal–organic framework host for sulfur storage in fast, long-cycle Li–S batteries

Junwen Zhou, Rui Li, Xinxin Fan, Yifa Chen, Ruodan Han, Wei Li, Jie Zheng, Bo Wang\* and Xingguo Li\*

A fast and stable sulfur cathode is achieved by using ZIF-8 nanocrystals as a host material with a small window size (3.4 Å) plus a small and uniform particle size (100–200 nm).

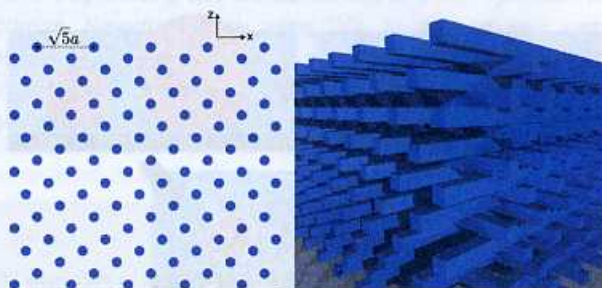


2725

### Light trapping in photonic crystals

Ken Xingze Wang, Zongfu Yu, Victor Liu, Aaswath Raman, Yi Cui and Shanhui Fan\*

We provide theoretical conditions for significant light-trapping enhancement in photonic crystals by explicitly relating the absorption enhancement to the density of states.

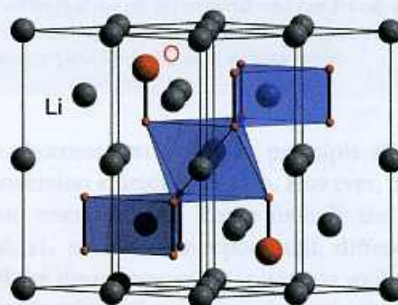


2739

### Short-range Li diffusion vs. long-range ionic conduction in nanocrystalline lithium peroxide Li<sub>2</sub>O<sub>2</sub>—the discharge product in lithium-air batteries

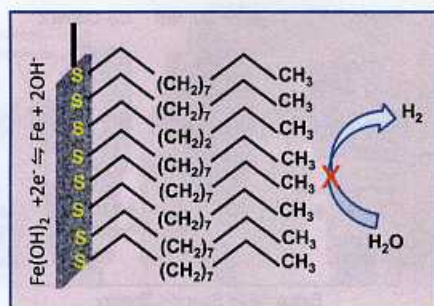
A. Dunst,\* V. Epp,\* I. Hanzu, S. A. Freunberger and M. Wilkening\*

Conductivity spectroscopy and <sup>7</sup>Li spin-locking NMR relaxometry reveal enhanced ion dynamics in nanocrystalline Li<sub>2</sub>O<sub>2</sub> prepared by high-energy ball milling.





2753

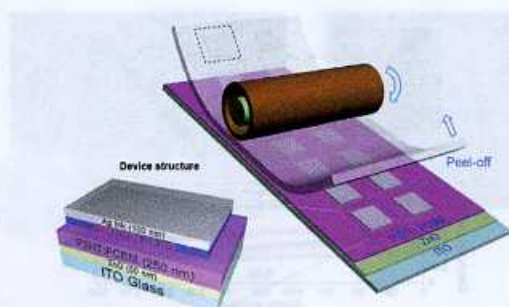


### Organo-sulfur molecules enable iron-based battery electrodes to meet the challenges of large-scale electrical energy storage

Bo Yang, Souradip Malkhandi, Aswin K. Manohar, G. K. Surya Prakash and S. R. Narayanan\*

An inexpensive, high-performance and robust rechargeable iron battery electrode has been demonstrated for large-scale electrical energy storage.

2764

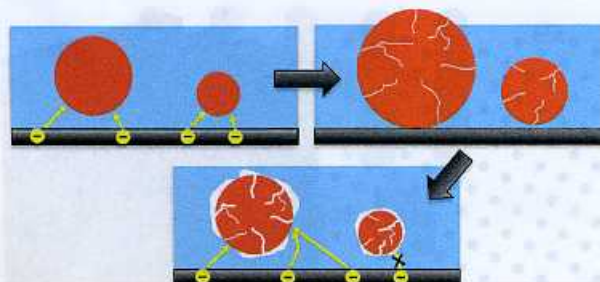


### Multi-film roll transferring (MRT) process using highly conductive and solution-processed silver solution for fully solution-processed polymer solar cells

Hongseok Youn, Taehwa Lee and L. Jay Guo\*

A multi-layer roll transferring (MRT) approach is reported, in which a highly conductive solution processed Ag electrode is prepared separately from the rest of the organic layers, and the fully solution-processed device is completed by a final roll-transferring process.

2771



### In situ nanotomography and operando transmission X-ray microscopy of micron-sized Ge particles

J. Nelson Weker,\* N. Liu, S. Misra, J. C. Andrews, Y. Cui and M. F. Toney\*

2D and 3D nanometer resolution imaging of Ge anodes during cycling show particle size-dependent fracturing and failure.