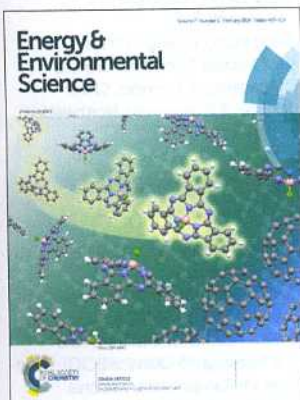


## IN THIS ISSUE

ISSN 1754-5692 CODEN EESNBY 7(2) 469–832 (2014)



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See Menke and Holmes,  
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Aspuru-Guzik *et al.*,  
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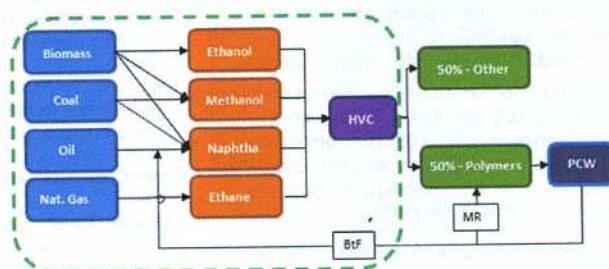
## ANALYSIS

482

### Energy demand and emissions of the non-energy sector

Vassilis Daioglou,\* Andre P. C. Faaij, Deger Saygin,  
Martin K. Patel, Birka Wicke and Detlef P. van Vuuren

The description and application of a model projecting energy demand and emissions of chemical feedstocks and the effect of mitigating measures.



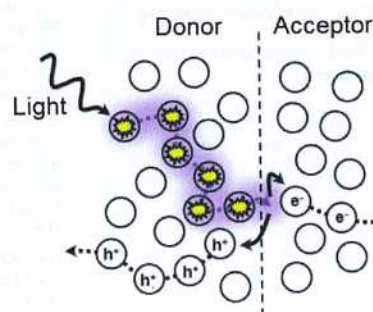
## REVIEWS

499

### Exciton diffusion in organic photovoltaic cells

S. Matthew Menke and Russell J. Holmes\*

The efficient harvesting of excitons is an essential step in the operation of organic photovoltaic cells. The ability to engineer and tailor exciton transport remains a key challenge for the design of next generation devices. In this review, we examine recent efforts to characterize exciton transport as well as novel material and device-based techniques aimed at extending the distance over which an exciton can migrate.

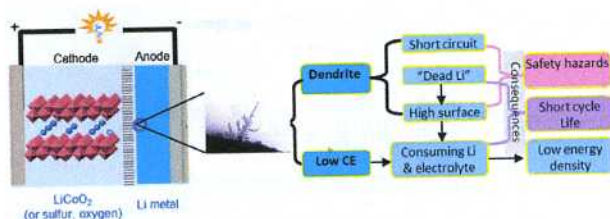


513

### Lithium metal anodes for rechargeable batteries

Wu Xu,\* Jiulin Wang, Fei Ding, Xilin Chen, Eduard Nasybulin, Yaohui Zhang and Ji-Guang Zhang\*

Lithium metal is an ideal anode for rechargeable batteries if dendrite growth and low Coulombic efficiency problems can be overcome.

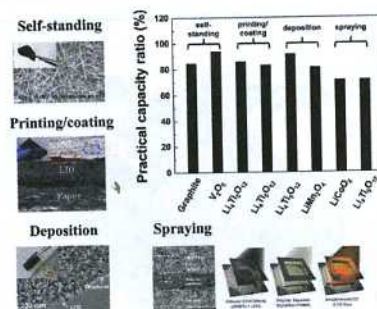


538

### Recent progress on flexible lithium rechargeable batteries

Hyeokjo Gwon, Jihyun Hong, Haegyeom Kim, Dong-Hwa Seo, Seokwoo Jeon and Kisuk Kang\*

This mini-review provides a comprehensive discussion of flexible lithium rechargeable battery technologies.

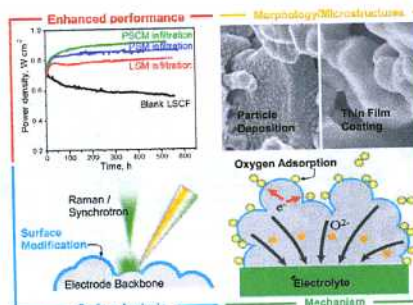


552

### Enhancing SOFC cathode performance by surface modification through infiltration

Dong Ding, Xiayi Li, Samson Yuxiu Lai, Kirk Gerdes and Meilin Liu\*

Wet chemical infiltration processes have been demonstrated to be effective to enhance electrocatalytic activity and stability in SOFC cathodes.

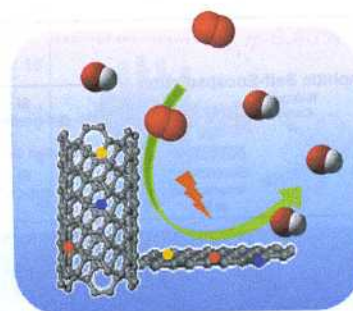


576

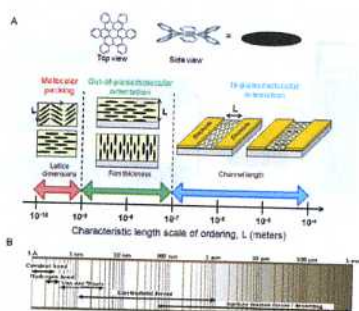
### Heterogeneous nanocarbon materials for oxygen reduction reaction

Da-Wei Wang\* and Dangsheng Su\*

This review updates the recent progress of heterogeneous nanocarbon electrocatalysts for the oxygen reduction reaction. The different functions of heteroatoms (N, O, B, P, S) and their combinations are revisited.







### Directing the film structure of organic semiconductors via post-deposition processing for transistor and solar cell applications

Anna M. Hiszpanski\* and Yueh-Lin Loo\*

Post-deposition processing methods offer means to control the structure of organic semiconductor thin films across various length scales.

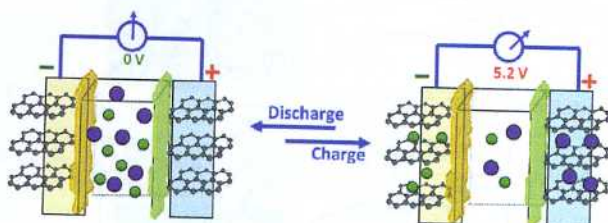
## COMMUNICATIONS



### High-performance bi-functional electrocatalysts of 3D crumpled graphene–cobalt oxide nanohybrids for oxygen reduction and evolution reactions

Shun Mao, Zhenhai Wen, Taizhong Huang, Yang Hou and Junhong Chen\*

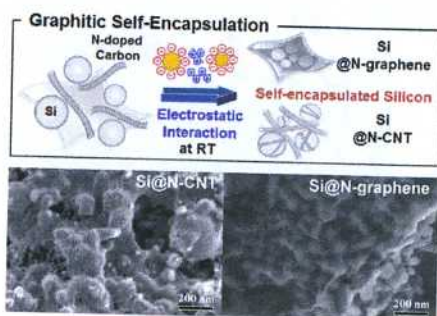
High-performance bi-functional electrocatalysts for oxygen reduction and evolution reactions were fabricated with 3D crumpled graphene–CoO hybrids.



### Dual-graphite chemistry enabled by a high voltage electrolyte

Jeffrey A. Read,\* Arthur V. Cresce, Matthew H. Ervin and Kang Xu

Schematic illustration of a dual-graphite intercalation cell wherein  $\text{Li}^+$  and  $\text{PF}_6^-$  are simultaneously accommodated in graphitic structures at the anode and cathode upon charge.



### N-doped graphitic self-encapsulation for high performance silicon anodes in lithium-ion batteries

Won Jun Lee, Tae Hoon Hwang, Jin Ok Hwang, Hyun Wook Kim, Joonwon Lim, Hu Young Jeong, Jongwon Shim, Tae Hee Han, Je Young Kim, Jang Wook Choi\* and Sang Ouk Kim\*

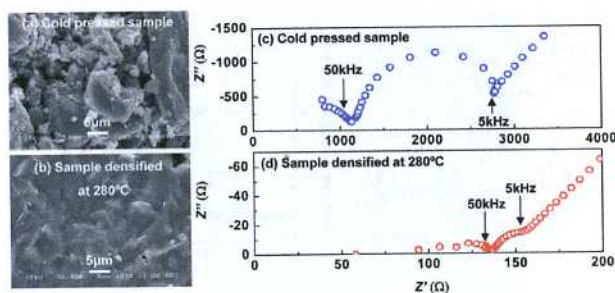
We demonstrate spontaneous room temperature graphitic encapsulation of Si particles for high performance LIB anodes with carbon nanotubes and graphene. Superior capacity retention and excellent rate capability have been achieved.

627

### A sulphide lithium super ion conductor is superior to liquid ion conductors for use in rechargeable batteries

Yoshikatsu Seino,\* Tsuyoshi Ota, Kazunori Takada, Akitoshi Hayashi and Masahiro Tatsumisago

We report that a heat-treated  $\text{Li}_2\text{S}-\text{P}_2\text{S}_5$  glass-ceramic conductor has an extremely high ionic conductivity of  $1.7 \times 10^{-2} \text{ S cm}^{-1}$  and the lowest conduction activation energy of  $17 \text{ kJ mol}^{-1}$  at room temperature among lithium-ion conductors reported to date.

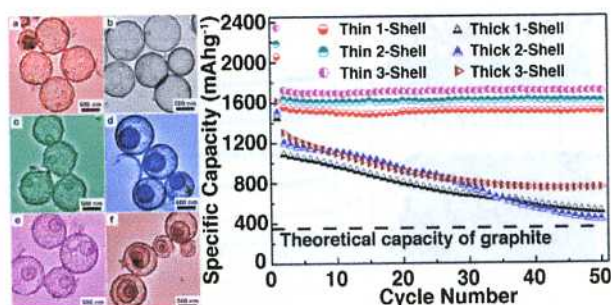


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### $\alpha\text{-Fe}_2\text{O}_3$ multi-shelled hollow microspheres for lithium ion battery anodes with superior capacity and charge retention

Simeng Xu, Colin M. Hessel, Hao Ren, Ranbo Yu,\* Quan Jin, Mei Yang, Huijun Zhao and Dan Wang\*

Multi-shelled  $\alpha\text{-Fe}_2\text{O}_3$  hollow microspheres show a thickness dependent lithium storage capacity of up to  $1702 \text{ mA h g}^{-1}$  at a current density of  $50 \text{ mA g}^{-1}$ .

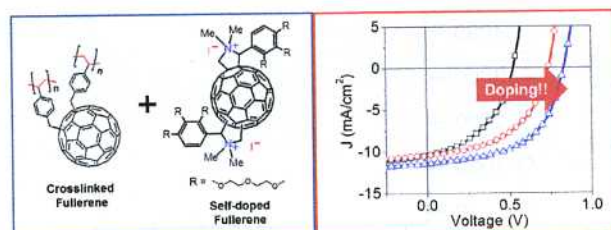


638

### In situ doping and crosslinking of fullerenes to form efficient and robust electron-transporting layers for polymer solar cells

Namchul Cho, Chang-Zhi Li, Hin-Lap Yip and Alex K.-Y. Jen\*

Efficient electron-transporting layers (ETLs) with a stable conductive fullerene doped into a thermally crosslinkable fullerene matrix have been developed for inverted polymer solar cells (PSCs).

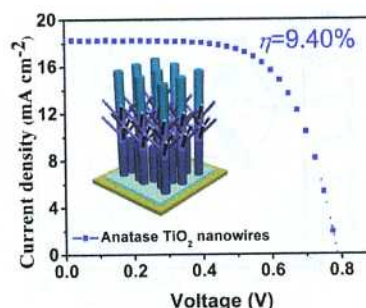


644

### Ultra-long anatase $\text{TiO}_2$ nanowire arrays with multi-layered configuration on FTO glass for high-efficiency dye-sensitized solar cells

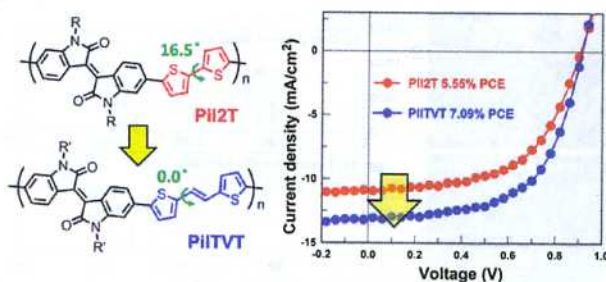
Wu-Qiang Wu, Yang-Fan Xu, Cheng-Yong Su and Dai-Bin Kuang\*

DSSC based on  $47 \mu\text{m}$ -long anatase  $\text{TiO}_2$  nanowire array attains an impressive power conversion efficiency of 9.40%.





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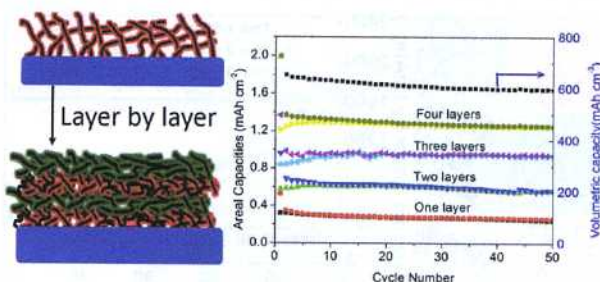


# $\pi$ -Extended low bandgap polymer based on isoindigo and thienylvinylene for high performance polymer solar cells

Eui Hyuk Jung and Won Ho Jo\*

A  $\pi$ -extended low bandgap polymer, PI1TVT showed a promising power conversion efficiency of 7.09% in polymer solar cells. It is higher than that of PI12T (5.55%), because of the better coplanar structure of the TVT unit than the 2T unit.

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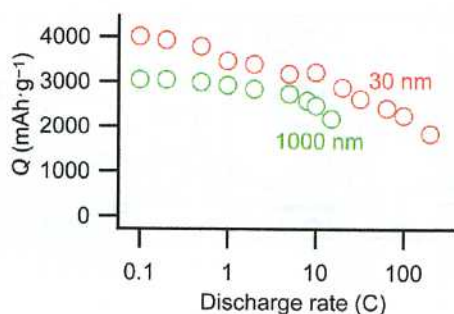


# A multilayer Si/CNT coaxial nanofiber LIB anode with a high areal capacity

Qizhen Xiao, Yu Fan, Xinghui Wang, Rahmat Agung Susantyoko and Qing Zhang\*

Multilayer Si/CNT composites have been used as LIB anodes, which have significantly high silicon loading, areal capacity and excellent cyclability.

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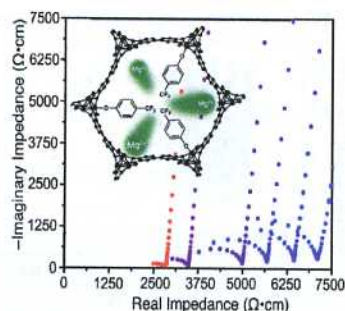


# High performance silicon-based anodes in solid-state lithium batteries

Rinlee B. Cervera, Naoki Suzuki, Tsuyoshi Ohnishi, Minoru Osada, Kazutaka Mitsuishi, Takayoshi Kambara and Kazunori Takada\*

Si-based anodes fabricated into thin films exhibit high capacity and rate capability in a solid electrolyte.

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# Metal-organic frameworks as solid magnesium electrolytes

M. L. Aubrey, R. Ameloot, B. M. Wiers and J. R. Long\*

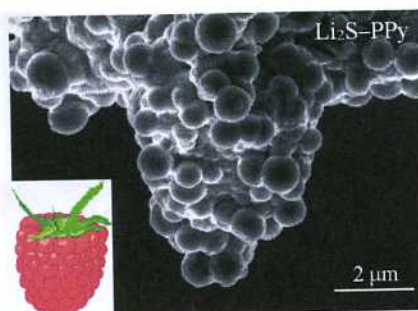
By post-synthetic modification of a metal-organic framework, solid magnesium electrolytes have been prepared with room temperature ionic conductivities over one-hundred times greater than any previously reported rigid material.

672

# Facile synthesis of $\text{Li}_2\text{S}$ -polypyrrole composite structures for high-performance $\text{Li}_2\text{S}$ cathodes

Zhi Wei Seh, Haotian Wang, Po-Chun Hsu, Qianfan Zhang, Weiyang Li, Guangyuan Zheng, Hongbin Yao and Yi Cui\*

We report *in situ* synthesis of  $\text{Li}_2\text{S}$ -polypyrrole composite cathodes with favorable Li-N interaction for stable cycling performance.

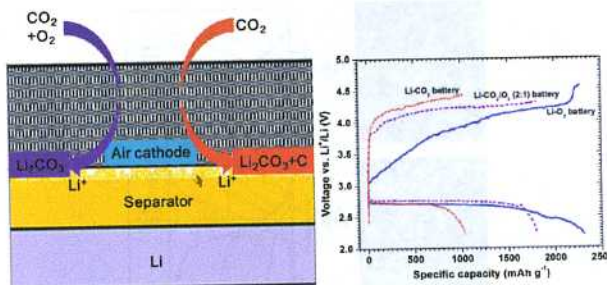


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# Rechargeable $\text{Li}/\text{CO}_2\text{-O}_2$ (2 : 1) battery and $\text{Li}/\text{CO}_2$ battery

Yali Liu, Rui Wang, Yingchun Lyu, Hong Li\* and Liqun Chen

Rechargeable  $\text{Li}/\text{CO}_2\text{-O}_2$  (2 : 1, volume ratio) battery and a rechargeable  $\text{Li}/\text{CO}_2$  battery are reported.  $\text{Li}_2\text{CO}_3$  is the main product for both batteries.

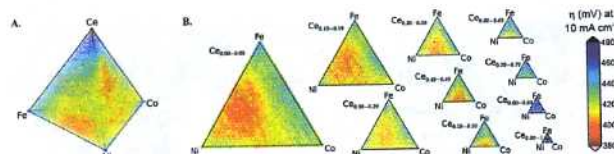


682

# Discovering Ce-rich oxygen evolution catalysts, from high throughput screening to water electrolysis

Joel A. Haber, Yun Cai, Suho Jung, Chengxiang Xiang, Slobodan Mitrovic, Jian Jin, Alexis T. Bell and John M. Gregoire\*

We report a new Ce-rich family of active oxygen evolution reaction (OER) catalysts composed of earth abundant elements, discovered using high-throughput methods.

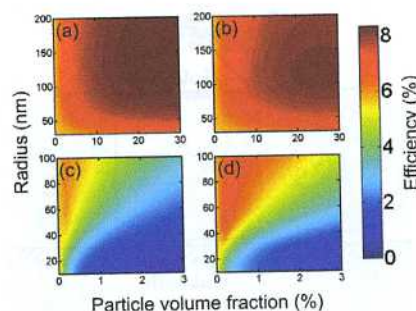


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# Dye sensitized solar cells as optically random photovoltaic media

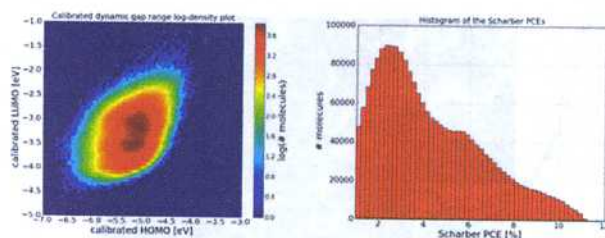
Francisco Enrique Gálvez, Piers R. F. Barnes, Janne Halme and Hernán Míguez\*

We theoretically analyze dye solar cells, in which different kinds of spherical scattering particles have been added to the absorbing electrode, as random optical media, a design rule being found to optimize their performance.





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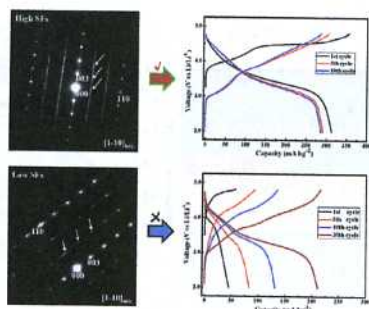


### Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry – the Harvard Clean Energy Project

J. Hachmann,\* R. Olivares-Amaya, A. Jinich, A. L. Appleton, M. A. Blood-Forsythe, L. R. Seress, C. Román-Salgado, K. Trepte, S. Atahan-Evrenk, S. Er, S. Shrestha, R. Mondal, A. Sokolov, Z. Bao and A. Aspuru-Guzik\*

We present a virtual high-throughput screening of organic semiconductors to identify lead candidates for photovoltaic materials, and extract patterns of their structural makeup.

705

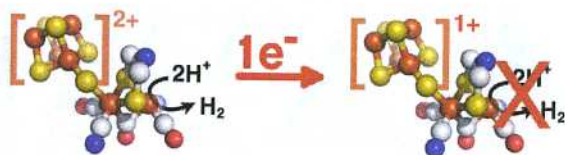


### Improving the electrochemical performance of layered lithium-rich transition-metal oxides by controlling the structural defects

Jinlong Liu, Mengyan Hou, Jin Yi, Shaoshuai Guo, Congxiao Wang and Yongyao Xia\*

The amount of stacking faults (SFs) in the  $\text{Li}_2\text{MnO}_3$  component plays a crucial role in the electrochemistry of  $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$  electrodes.

715

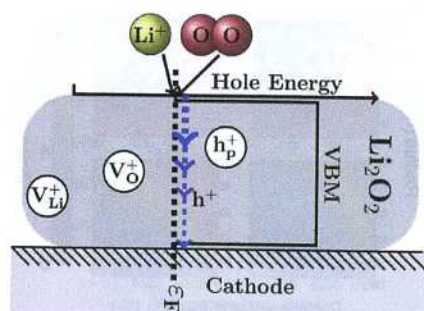


### FeFe hydrogenase reductive inactivation and implication for catalysis

Viviane Hajj, Carole Baffert, Kateryna Sybirna, Isabelle Meynial-Salles, Philippe Soucaille, Hervé Bottin, Vincent Fourmond and Christophe Léger\*

The demonstration that FeFe hydrogenases inactivate at low potential changes the way we think about their mechanism and their use in solar  $\text{H}_2$  production.

720



### Lithium and oxygen vacancies and their role in $\text{Li}_2\text{O}_2$ charge transport in Li– $\text{O}_2$ batteries

J. B. Varley, V. Viswanathan, J. K. Nørskov and A. C. Luntz\*

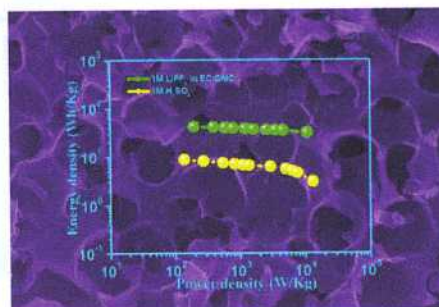
This paper determines the formation energy of polarons and vacancies in  $\text{Li}_2\text{O}_2$  as it is electrochemically forming and shows how they affect charge transport through  $\text{Li}_2\text{O}_2$ .

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### 3D micro-porous conducting carbon beehive by single step polymer carbonization for high performance supercapacitors: the magic of *in situ* porogen formation

Dhanya Puthusseri, Vanchiappan Aravindan, Srinivasan Madhavi and Satishchandra Ogale\*

High surface area 3D conducting carbon with beehive morphology derived by single step pyrolysis of selected polymer shows excellent performance as supercapacitor electrode.

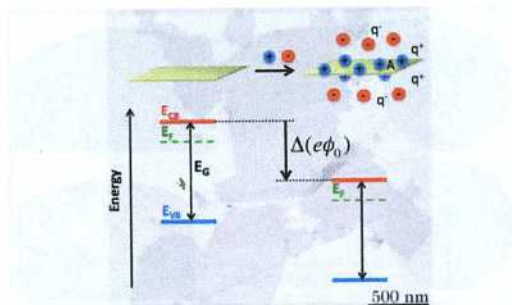


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### Use of potential determining ions to control energetics and photochemical charge transfer of a nanoscale water splitting photocatalyst

Rachel L. Chamousis and Frank E. Osterloh\*

Specifically adsorbed ions modify the energetics and photoelectrocatalytic properties of nanocrystals.

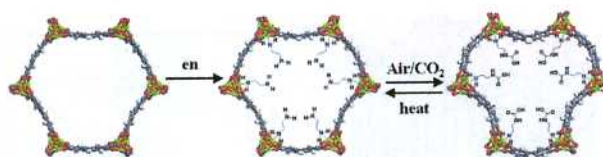


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### Diamine-functionalized metal-organic framework: exceptionally high CO<sub>2</sub> capacities from ambient air and flue gas, ultrafast CO<sub>2</sub> uptake rate, and adsorption mechanism

Woo Ram Lee, Sang Yeon Hwang, Dae Won Ryu, Kwang Soo Lim, Sang Soo Han, Dohyun Moon, Jungkyu Choi and Chang Seop Hong\*

A framework en-Mg<sub>2</sub>(dobpdc) functionalized with ethylenediamine exhibits a record high CO<sub>2</sub> capacity from air (0.39 mbar) with potential for application in CO<sub>2</sub> capture.

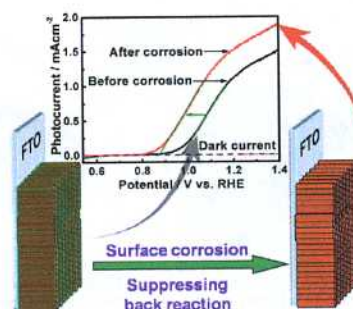


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### Cathodic shift of onset potential for water oxidation on a Ti<sup>4+</sup> doped Fe<sub>2</sub>O<sub>3</sub> photoanode by suppressing the back reaction

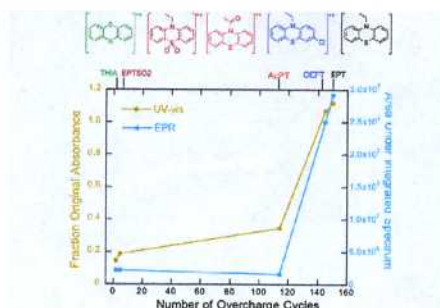
Dapeng Cao, Wenjun Luo,\* Jianyong Feng, Xin Zhao, Zhaosheng Li and Zhigang Zou\*

Suppressing the back reaction caused an about 100 mV cathodic shift of the photocurrent onset potential on a hematite photoanode.





760

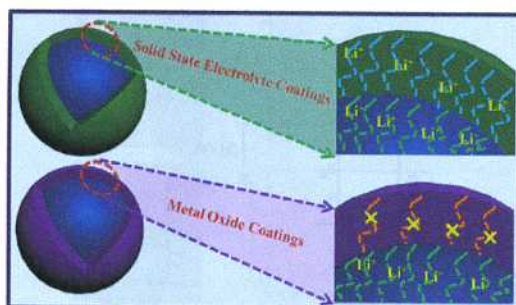


### A fast, inexpensive method for predicting overcharge performance in lithium-ion batteries

Susan A. Odom,\* Selin Ergun, Pramod P. Poudel and Sean R. Parkin

The stability of the radical cations of a series of related aromatic heterocycles – as measured by UV-vis and EPR spectroscopy – shows a correlation to the number of overcharge cycles in lithium-ion batteries.

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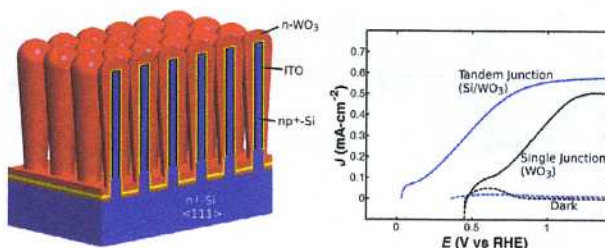


### Atomic layer deposition of solid-state electrolyte coated cathode materials with superior high-voltage cycling behavior for lithium ion battery application

Xifei Li, Jian Liu, Mohammad Norouzi Banis, Andrew Lushington, Ruying Li, Mei Cai and Xueliang Sun\*

A highly lithium ionic conductive solid-state electrolyte coating layer significantly increases cathode performance in lithium ion batteries.

779

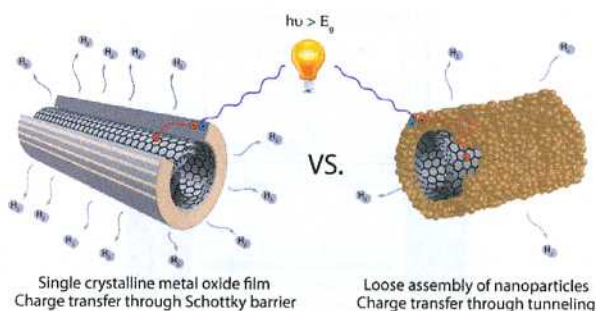


### Photoelectrochemistry of core-shell tandem junction n-p+-Si/n-WO<sub>3</sub> microwire array photoelectrodes

Matthew R. Shaner, Katherine T. Fountaine, Shane Ardo, Rob H. Coridan, Harry A. Atwater and Nathan S. Lewis\*

A demonstration of an integrated Si/WO<sub>3</sub> microwire array tandem junction device for photoelectrochemical water splitting.

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### Interface engineering in nanocarbon-Ta<sub>2</sub>O<sub>5</sub> hybrid photocatalysts

Alexey S. Cherevan, Paul Gebhardt, Cameron J. Shearer, Michinori Matsukawa, Kazunari Domen and Dominik Eder\*

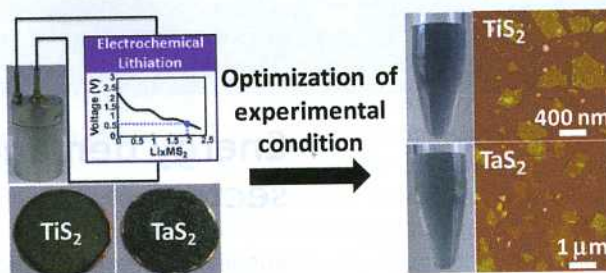
We demonstrate a new hybrid morphology that facilitates charge transport and charge separation at the interface between the nanocarbon and the semiconductor and so greatly improves their performance in environmental and sustainable energy applications.

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### Growth of noble metal nanoparticles on single-layer $\text{TiS}_2$ and $\text{TaS}_2$ nanosheets for hydrogen evolution reaction

Zhiyuan Zeng, Chaoliang Tan, Xiao Huang, Shuyu Bao and Hua Zhang\*

Single-layer  $\text{TiS}_2$  and  $\text{TaS}_2$  nanosheets functionalized with Pt and Au nanoparticles exhibit good electrocatalytic activity towards hydrogen evolution reaction.

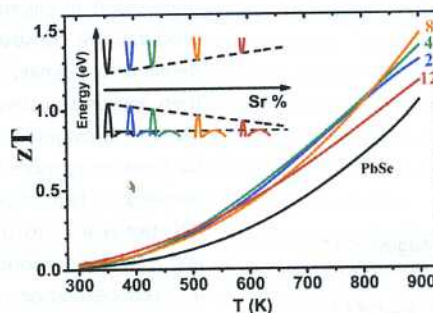


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### Tuning bands of $\text{PbSe}$ for better thermoelectric efficiency

Heng Wang,\* Zachary M. Gibbs, Yoshiki Takagiwa and G. Jeffrey Snyder\*

Improving the thermoelectric performance of  $\text{PbSe}$  over its previously reported maximum  $zT$  can be achieved by engineering its electronic band structure.

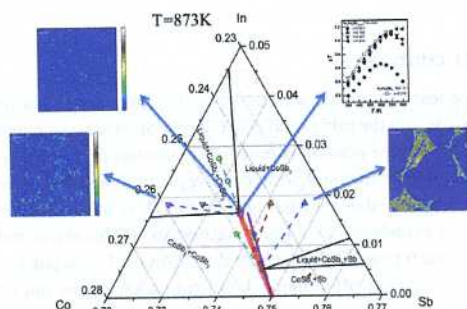


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### Phase diagram of $\text{In-Co-Sb}$ system and thermoelectric properties of $\text{In}$ -containing skutterudites

Yinglu Tang, Yuting Qiu, Lili Xi, Xun Shi,\* Wenqing Zhang, Lidong Chen, Ssu-Ming Tseng, Sinn-wen Chen and G. Jeffrey Snyder\*

The isothermal section of ternary phase diagram of  $\text{In-Co-Sb}$  system at 873 K explains the solubility debate of  $\text{In}$  in skutterudite.



820

### Oxygen evolution catalysts on supports with a 3-D ordered array structure and intrinsic proton conductivity for proton exchange membrane steam electrolysis

Junyuan Xu, David Aili, Qingfeng Li,\* Erik Christensen, Jens Oluf Jensen, Wei Zhang, Martin Kalmar Hansen, Gaoyang Liu, Xindong Wang\* and Niels J. Bjerrum

Three-dimensionally ordered hexagonal array supports with mixed conductivities are synthesized containing phosphates and tin doped indium oxides for OER catalysts.

