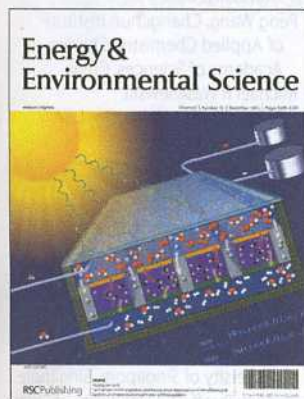


## IN THIS ISSUE

ISSN 1754-5692 CODEN EESNBY 6(12) 3389–3794 (2013)



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See Haussener *et al.*,  
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**Inside cover**  
See Lou *et al.*, pp. 3619–3626.  
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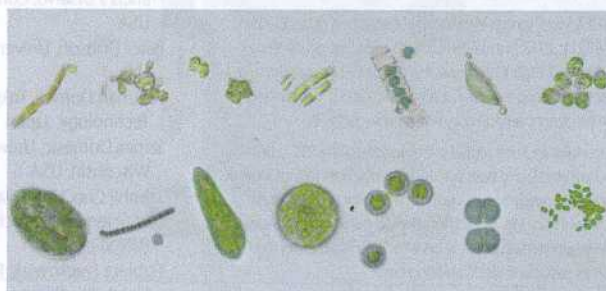
## OPINION

3404

### Survival of the fattest

Peter R. Mooij,\* Gerben R. Stouten, Jelmer Tamis,  
Mark C. M. van Loosdrecht and Robbert Kleerebezem

By creating a selective environment we show how to obtain  
a stable and open system, populated by highly productive  
microalgae.



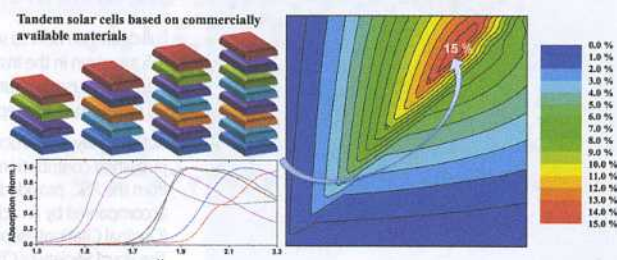
## ANALYSIS

3407

### Towards 15% energy conversion efficiency: a systematic study of the solution-processed organic tandem solar cells based on commercially available materials

Ning Li,\* Derya Baran, Karen Forberich, Florian Machui,  
Tayebeh Ameri, Mathieu Turbiez,  
Miguel Carrasco-Orozco, Martin Drees, Antonio Facchetti,  
Frederik C. Krebs and Christoph J. Brabec

A PCE of 15% becomes possible for organic tandem solar  
cells based on commercially available donor materials.

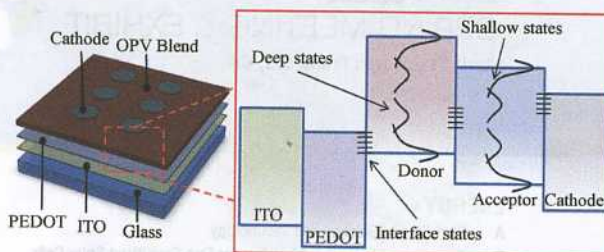


3414

**The identification, characterization and mitigation of defect states in organic photovoltaic devices: a review and outlook**

John A. Carr and Sumit Chaudhary\*

This report comprehensively reviews the identification, characterization, mitigation and effects of electronic defect levels in organic photovoltaic devices.

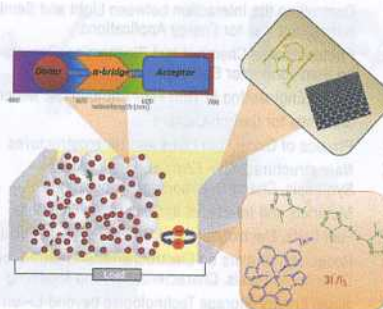


3439

**Metal free sensitizer and catalyst for dye sensitized solar cells**

Shahzada Ahmad,\* Elena Guillén, Ladislav Kavan, Michael Grätzel and Mohammad K. Nazeeruddin

Cost reduction: Towards metal free dye sensitized solar cells.

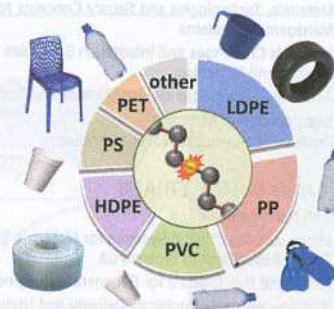


3467

**Retrieving and converting energy from polymers: deployable technologies and emerging concepts**

Bilge Baytekin, H. Tarik Baytekin and Bartosz A. Grzybowski\*

Significant amounts of energy can be retrieved from polymers via approaches ranging from incineration, to thermolysis, to mechanochemistry and thermoelectricity.

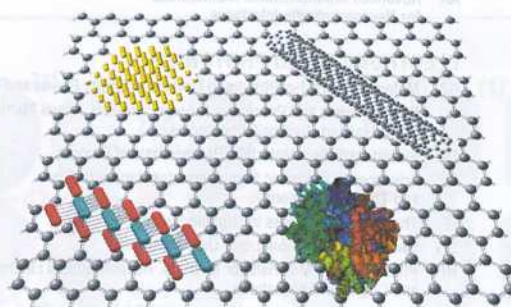


3483

**Graphene-based nanocomposites: preparation, functionalization, and energy and environmental applications**

Haixin Chang\* and Hongkai Wu\*

Graphene nanocomposites with controlled functionalizations and physical and chemical properties provide unique opportunities for energy and environmental science.

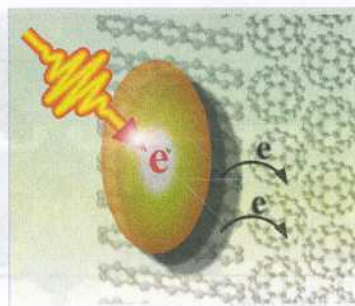


3508

### Exceeding the Shockley–Queisser limit in solar energy conversion

Cory A. Nelson, Nicholas R. Monahan and X.-Y. Zhu\*

Photophysical mechanisms in molecular and nano materials for solar energy conversion beyond the Shockley–Queisser limit.

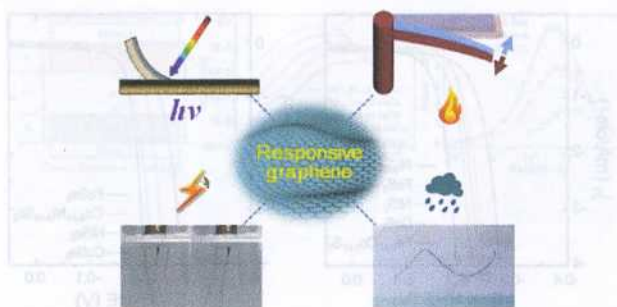


3520

### Stimulus-responsive graphene systems towards actuator applications

Yang Zhao, Long Song, Zhipan Zhang\* and Liangti Qu\*

Smart graphene systems respond to external stimuli for actuator applications.



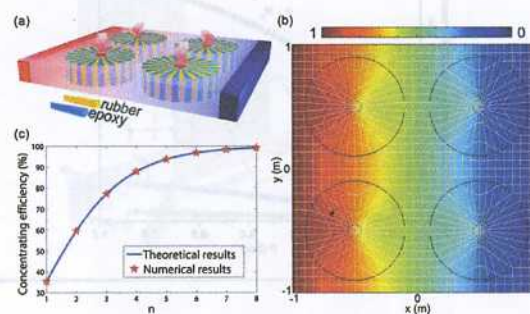
## COMMUNICATIONS

3537

### Theoretical realization of an ultra-efficient thermal-energy harvesting cell made of natural materials

Tiancheng Han, Jiajun Zhao, Tao Yuan, Dang Yuan Lei, Baowen Li and Cheng-Wei Qiu\*

An ultra-efficient thermal-energy harvesting cell made of natural materials.

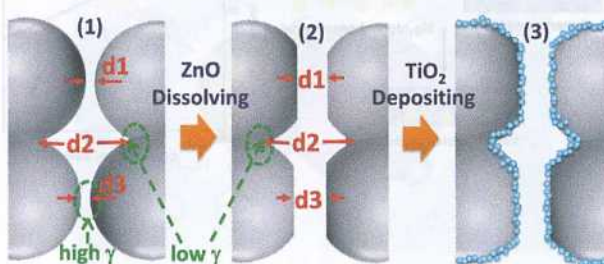


3542

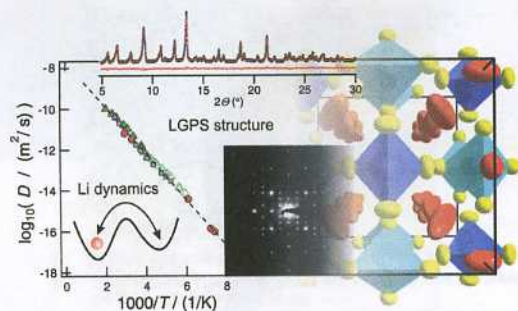
### Architected ZnO photoelectrode for high efficiency quantum dot sensitized solar cells

Jianjun Tian,\* Qifeng Zhang, Evan Uchaker, Rui Gao, Xuanhui Qu, Shengen Zhang and Guozhong Cao\*

A CdS/CdSe quantum dot sensitized solar cell assembled with a ZnO photoelectrode with efficiency of 4.68% was obtained by a facile chemical passivation process.



3548

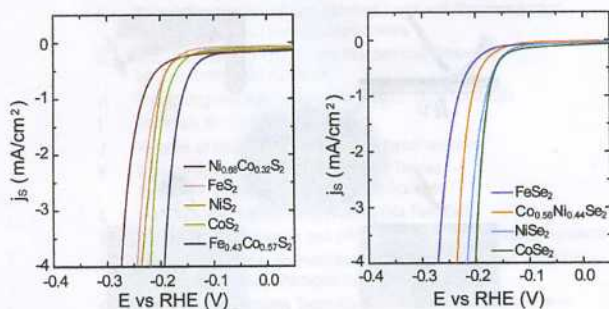


### Tetragonal $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ and $\text{Li}_7\text{GePS}_8$ – exploring the Li ion dynamics in LGPS Li electrolytes

Alexander Kuhn, Viola Duppel and Bettina V. Lotsch\*

Characterization of the structure and ultrafast Li ion dynamics of the LGPS electrolytes  $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$  and  $\text{Li}_7\text{GePS}_8$ .

3553

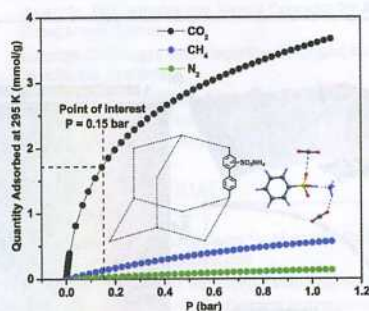


### First-row transition metal dichalcogenide catalysts for hydrogen evolution reaction

Desheng Kong, Judy J. Cha, Haotian Wang, Hye Ryoung Lee and Yi Cui\*

A group of first-row transition metal dichalcogenides are shown to be active catalysts for the hydrogen evolution reaction in an acidic electrolyte.

3559

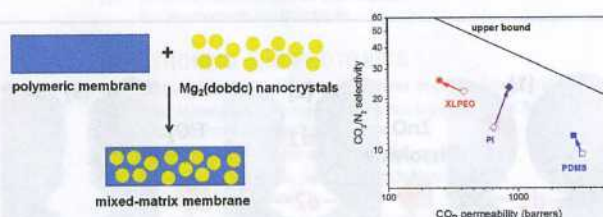


### Building multiple adsorption sites in porous polymer networks for carbon capture applications

Weigang Lu, Wolfgang M. Verdegaal, Jiamei Yu, Perla B. Balbuena, Hae-Kwon Jeong and Hong-Cai Zhou\*

A porous polymer network with multiple adsorption sites boosts  $\text{CO}_2$  capacity at low pressures and selectivity over other gas molecules.

3565



### $\text{CO}_2/\text{N}_2$ separations with mixed-matrix membranes containing $\text{Mg}_2(\text{dobdc})$ nanocrystals

Tae-Hyun Bae and Jeffrey R. Long\*

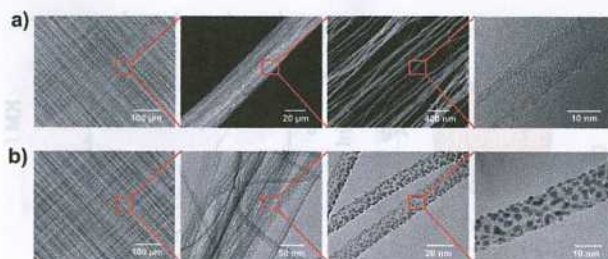
The  $\text{CO}_2/\text{N}_2$  separation performance of a polymer membrane was improved by incorporating nanocrystals of the metal-organic framework  $\text{Mg}_2(\text{dobdc})$  within a glassy polymer with a rigid backbone structure that restricts pore plugging.

3570

### A new catalyst-embedded hierarchical air electrode for high-performance Li-O<sub>2</sub> batteries

Hee-Dae Lim, Hyelynn Song, Hyeokjo Gwon, Kyu-Young Park, Jinsoo Kim, Youngjoon Bae, Hyungsub Kim, Sung-Kyun Jung, Taewoo Kim, Yong Hyup Kim, Xavier Lepró, Raquel Ovalle-Robles, Ray H. Baughman and Kisuk Kang\*

The Li-O<sub>2</sub> battery holds great promise as an ultra-high-energy-density device.

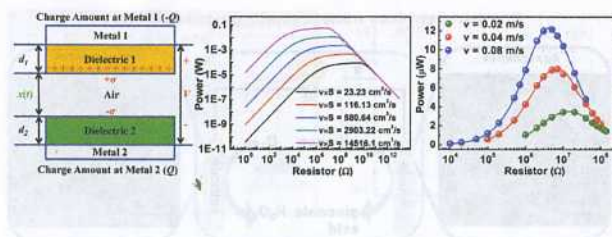


3576

### Theoretical study of contact-mode triboelectric nanogenerators as an effective power source

Simiao Niu, Sihong Wang, Long Lin, Ying Liu, Yu Sheng Zhou, Youfan Hu and Zhong Lin Wang\*

The first comprehensive theoretical model for contact-mode triboelectric nanogenerators is provided, which can serve as important guidance for their rational design.

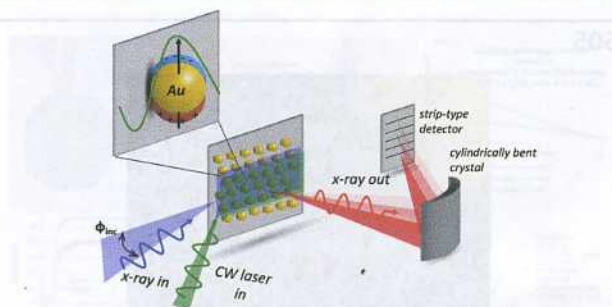


3584

### Direct observation of charge separation on Au localized surface plasmons

Jacinto Sá,\* Giulia Tagliabue, Peter Friedli, Jakub Szlachetko, Mercedes H. Rittmann-Frank, Fabio G. Santomauro, Christopher J. Milne and Hans Sigg

Plasmonic nano-structures of d<sup>10</sup> metals are suggested to be the future of photo-voltaics and photo-catalysis under solar irradiation, thanks to their large light absorption cross-section, versatility, and stability.

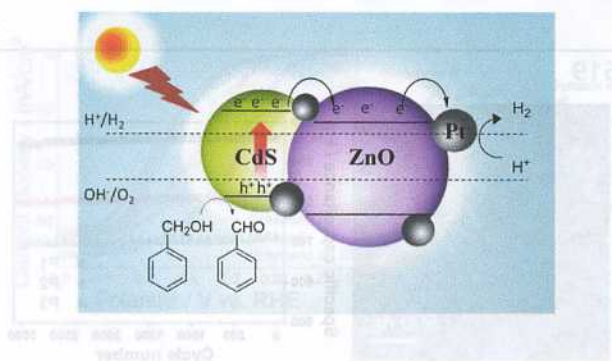


3589

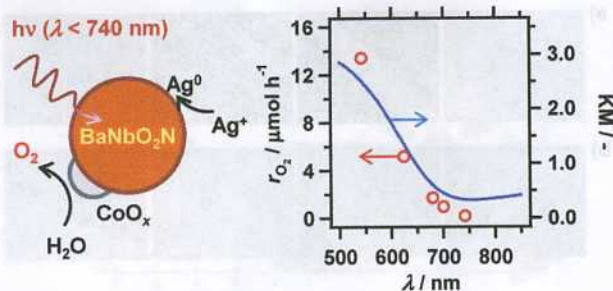
### Highly efficient photocatalytic hydrogen generation by solution-processed ZnO/Pt/CdS, ZnO/Pt/Cd<sub>1-x</sub>Zn<sub>x</sub>S and ZnO/Pt/CdS<sub>1-x</sub>Se<sub>x</sub> hybrid nanostructures

S. R. Lingampalli, Ujjal K. Gautam and C. N. R. Rao\*

Excellent hydrogen generation has been achieved by employing hybrid nanostructures of the type ZnO/Pt/Cd<sub>1-x</sub>Zn<sub>x</sub>S (CdS<sub>1-x</sub>Se<sub>x</sub>) prepared by simple solution processing.



3595



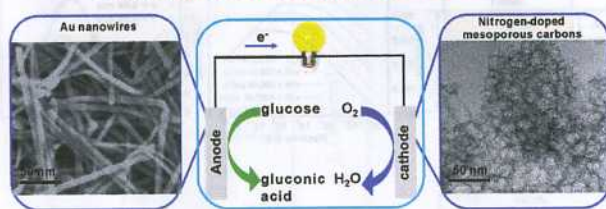
### Photocatalytic oxygen evolution using $\text{BaNbO}_2\text{N}$ modified with cobalt oxide under photoexcitation up to 740 nm

Takashi Hisatomi, Chisato Katayama, Yosuke Moriya, Tsutomu Minegishi, Masao Katayama, Hiroshi Nishiyama, Taro Yamada and Kazunari Domen\*

$\text{BaNbO}_2\text{N}$  loaded with a  $\text{CoO}_x$  cocatalyst generated oxygen from an aqueous  $\text{AgNO}_3$  solution under illumination up to 740 nm.

3600

### Compartment-less nonenzymatic glucose-air fuel cell



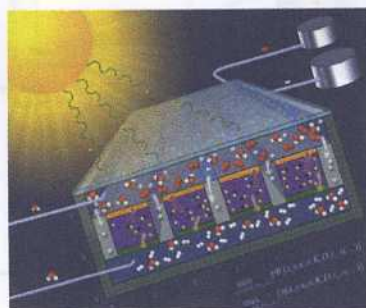
### A compartment-less nonenzymatic glucose-air fuel cell with nitrogen-doped mesoporous carbons and Au nanowires as catalysts

Mi Chu, Yijia Zhang, Lu Yang, Yueming Tan,\* Wenfang Deng, Ming Ma, Xiaoli Su, Qingji Xie\* and Shouzhuo Yao

A high-performance compartment-less glucose-air fuel cell was constructed with Au nanowires and nitrogen-doped mesoporous carbons as anodic and cathodic catalysts, respectively.

## PAPERS

3605

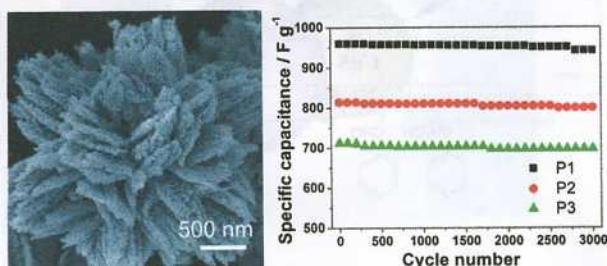


### Simulations of the irradiation and temperature dependence of the efficiency of tandem photoelectrochemical water-splitting systems

Sophia Haussener,\* Shu Hu, Chengxiang Xiang, Adam Z. Weber and Nathan S. Lewis\*

A multi-physics computational model has been used to simulate the efficiency of tandem photoelectrochemical water-splitting systems and to investigate the efficiency changes in response to variations in operational conditions (irradiation, concentration, and temperature) and the system's component characteristics.

3619



### Facile synthesis of mesoporous $\text{Ni}_{0.3}\text{Co}_{2.7}\text{O}_4$ hierarchical structures for high-performance supercapacitors

Hao Bin Wu, Huan Pang\* and Xiong Wen (David) Lou\*

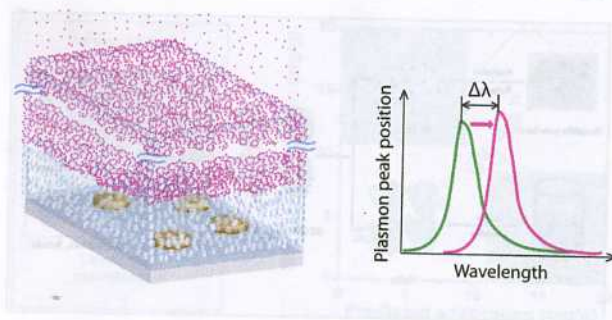
Mesoporous nickel cobalt oxide ( $\text{Ni}_{0.3}\text{Co}_{2.7}\text{O}_4$ ) hierarchical structures synthesized via a facile precipitation and thermal annealing approach exhibit excellent electrochemical performance for supercapacitors.

3627

### Diffusion and adsorption of dye molecules in mesoporous TiO<sub>2</sub> photoelectrodes studied by indirect nanoplasmonic sensing

Viktoria Gusak, Leo-Philipp Heiniger, Vladimir P. Zhdanov, Michael Grätzel, Bengt Kasemo and Christoph Langhammer\*

Using hidden-interface indirect nanoplasmonic sensing we scrutinize the dye molecule percolation process in dye sensitized solar cell TiO<sub>2</sub> photoelectrode mimics.

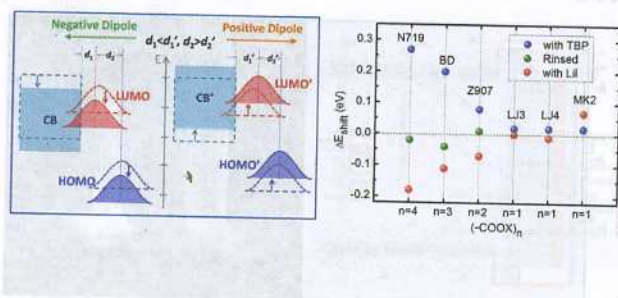


3637

### Coordinated shifts of interfacial energy levels: insight into electron injection in highly efficient dye-sensitized solar cells

Xudong Yang, Shufang Zhang, Kun Zhang, Jian Liu, Chuanjiang Qin, Han Chen, Ashraf Islam and Liyuan Han\*

An advanced understanding of the electron injection mechanism in highly efficient dye-sensitized solar cells has been reported based on findings of the realignment of interfacial energy levels and the redistribution of molecular orbitals.

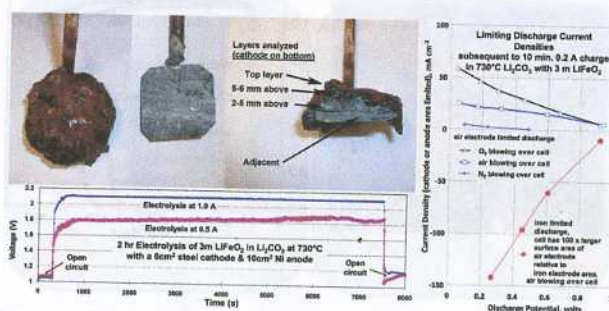


3646

### Molten air – a new, highest energy class of rechargeable batteries

Stuart Licht,\* Baochen Cui, Jessica Stuart, Baohui Wang and Jason Lau

This study introduces the principles of a new class of high-energy batteries and their fundamental chemistry is demonstrated.

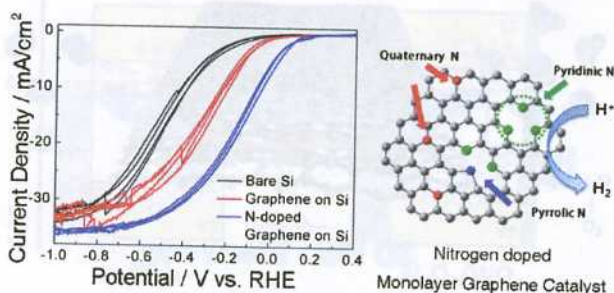


3658

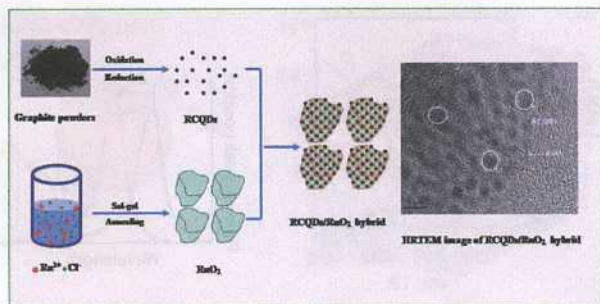
### N-doped monolayer graphene catalyst on silicon photocathode for hydrogen production

Uk Sim, Tae-Youl Yang, Joonhee Moon, Junghyun An, Jinyeon Hwang, Jung-Hye Seo, Jouhahn Lee, Kye Yeop Kim, Joohee Lee, Seungwu Han, Byung Hee Hong\* and Ki Tae Nam\*

The N-doped monolayer graphene on a silicon photoelectrode shows high catalytic activity for hydrogen production in an aqueous solution.



3665

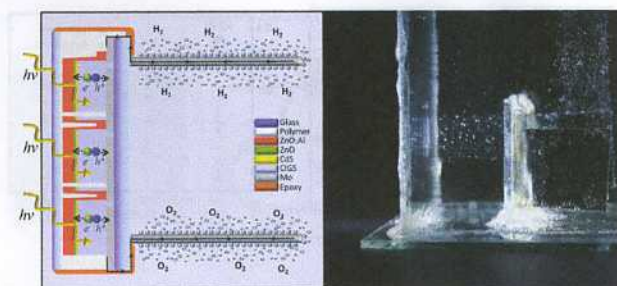


### A carbon quantum dot decorated RuO<sub>2</sub> network: outstanding supercapacitances under ultrafast charge and discharge

Yirong Zhu, Xiaobo Ji,\* Chenchi Pan, Qingqing Sun, Weixin Song, Laibing Fang, Qiyuan Chen and Craig E. Banks\*

A new carbon quantum dot-based hybrid as an excellent electrode material for supercapacitors is firstly and successfully fabricated with the composite exhibiting excellent electrochemical performances.

3676

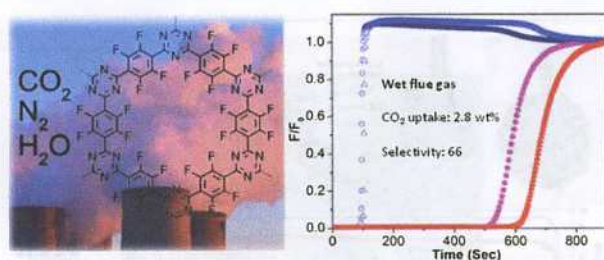


### A monolithic device for solar water splitting based on series interconnected thin film absorbers reaching over 10% solar-to-hydrogen efficiency

T. Jesper Jacobsson,\* Viktor Fjällström, Martin Sahlberg, Marika Edoff and Tomas Edvinsson

On the construction of a monolithic device for unassisted water splitting based on series interconnected CIGS cells reaching 10% efficiency.

3684

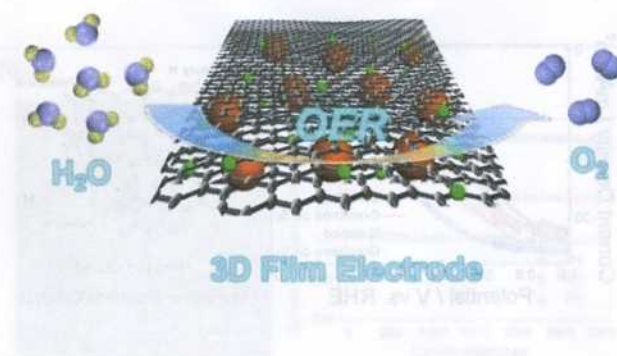


### A perfluorinated covalent triazine-based framework for highly selective and water-tolerant CO<sub>2</sub> capture

Yunfeng Zhao, Ke Xin Yao, Baiyang Teng, Tong Zhang and Yu Han\*

A perfluorinated covalent triazine-based framework exhibited excellent CO<sub>2</sub> adsorption and CO<sub>2</sub>-N<sub>2</sub> separation performance under both equilibrium and kinetic conditions, even in the presence of water.

3693



### N-doped graphene film-confined nickel nanoparticles as a highly efficient three-dimensional oxygen evolution electrocatalyst

Sheng Chen, Jingjing Duan, Jingrun Ran, Mietek Jaroniec and Shi Zhang Qiao\*

A novel 3D OER catalyst was fabricated by using N-doped graphene films as scaffolds and Ni nanoparticles as building blocks, which exhibited significantly enhanced catalytic performance with high activity, favorable kinetics and strong durability.

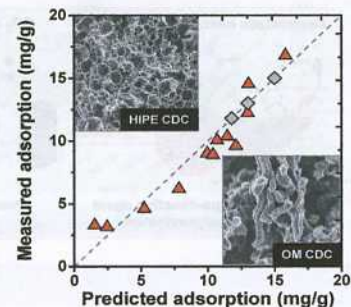
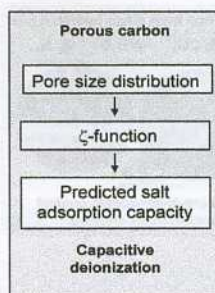


3700

### Direct prediction of the desalination performance of porous carbon electrodes for capacitive deionization

S. Porada, L. Borchardt, M. Oschatz, M. Bryjak, J. S. Atchison, K. J. Keesman, S. Kaskel, P. M. Biesheuvel and V. Presser\*

Desalination by capacitive deionization (CDI) is an emerging technology for the energy- and cost-efficient removal of ions from water by electrosorption in charged porous carbon electrodes.

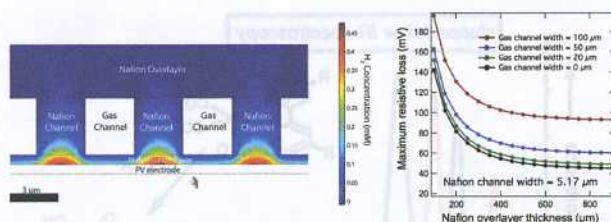


3713

### Modeling an integrated photoelectrolysis system sustained by water vapor

Chengxiang Xiang, Yikai Chen and Nathan S. Lewis\*

Multiphysics simulation of an integrated photoelectrolysis system sustained by water vapor or pure water.

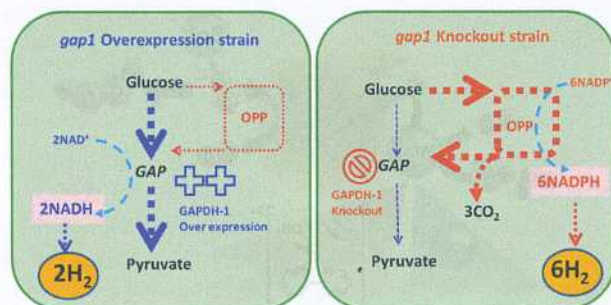


3722

### Reprogramming the glycolytic pathway for increased hydrogen production in cyanobacteria: metabolic engineering of NAD<sup>+</sup>-dependent GAPDH

G. Kenchappa Kumaraswamy, Tiago Guerra, Xiao Qian, Shuyi Zhang, Donald A. Bryant and G. Charles Dismukes\*

Metabolic engineering of GAPDH-1 of glycolysis and OPP pathways for increased NAD(P)H and hydrogen production, under dark-anoxic fermentative conditions.

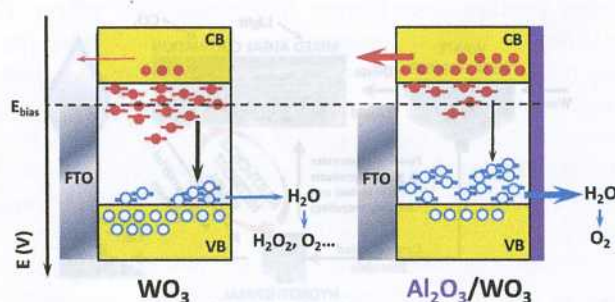


3732

### Promoting water photooxidation on transparent WO<sub>3</sub> thin films using an alumina overlayer

Wooyul Kim, Takashi Tachikawa, Damián Monllor-Satoca, Hyoung-il Kim, Tetsuro Majima and Wonyong Choi\*

In the water photooxidation process for the artificial photosynthesis, the alumina overlayer on a WO<sub>3</sub> photoanode markedly decreases the number of electron trapping sites, eventually facilitating the hole transfer to water.

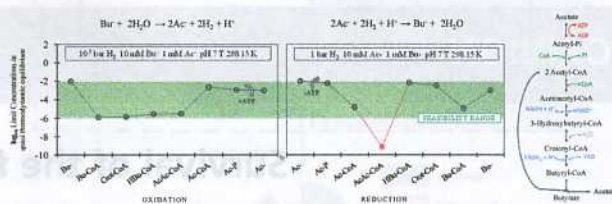




**Linking thermodynamics and kinetics to assess pathway reversibility in anaerobic bioprocesses**

Rebeca González-Cabaleiro,\* Juan M. Lema, Jorge Rodríguez and Robbert Kleerebezem

The reversibility of specific anaerobic metabolic pathways towards the production of reduced products is investigated by linking thermodynamics and kinetics.



**ADDITIONS AND CORRECTIONS**

**Additions and corrections published for 2013.**

For some time, storage compounds produced by photosynthetic microalgae are regarded as a potential resource for future fuel production. The main fuel precursors produced by algae are starch and triacylglycerol, whereas the precursors for biohydrogen, CH<sub>4</sub> or H<sub>2</sub> production whereas triacylglycerol is used as a precursor for biodiesel production. Since all algal species have different characteristics, some species produce more storage compounds than others. This explains the 'species-based' approach used in the majority of algal research: the choice of a species is regarded as a starting point for an experimental or process design. Unfortunately, storage compound production is not linearly related to the growth rate. Many productive strains either naturally occur that are genetically modified, are accompanied by faster growing algae when these are present in the system. A solution is to prevent other species from entering the system, as can be achieved in closed photobioreactors by sterilizing incoming and outgoing flows; however, sterilization comes at a cost, and maintaining a sterile monoculture is particularly troublesome. Some cultivation goals therefore require a certain risk to stable operation of a bioprocess.

Approximately 50 microbial strains are used for the majority of microalgae research, while a few billion years of evolution has resulted in 40 000 identified and a multitude of unidentified

microbial species. A 'strain-based' approach would be to select a species that is genetically modified to produce a specific storage compound. This approach would be similar to the 'species-based' approach used in the majority of algal research, but it would be more targeted. Unfortunately, storage compound production is not linearly related to the growth rate. Many productive strains either naturally occur that are genetically modified, are accompanied by faster growing algae when these are present in the system. A solution is to prevent other species from entering the system, as can be achieved in closed photobioreactors by sterilizing incoming and outgoing flows; however, sterilization comes at a cost, and maintaining a sterile monoculture is particularly troublesome. Some cultivation goals therefore require a certain risk to stable operation of a bioprocess.