

# Energy & Environmental Science

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## IN THIS ISSUE

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### Cover

See Chengxiang Xiang, Nathan S. Lewis, Harry A. Atwater *et al.*, pp. 3166-3172. Image reproduced by permission of Chengxiang Xiang from *Energy Environ. Sci.*, 2015, 8, 3166.



### Inside cover

See Yongchun Zhu, Yitai Qian *et al.*, pp. 3181-3186. Image reproduced by permission of Yongchun Zhu from *Energy Environ. Sci.*, 2015, 8, 3181.

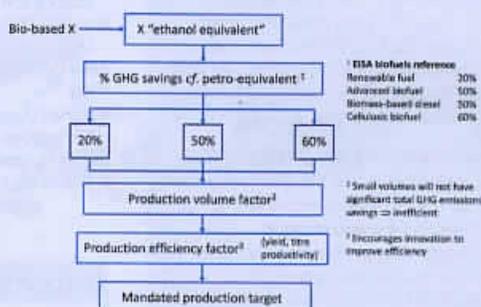
## OPINION

3063

### Balancing the bioeconomy: supporting biofuels and bio-based materials in public policy

Jim Philp

Key objectives for a bioeconomy are now embedded in the strategic activities of more than 30 countries, with an increasing number developing a national bioeconomy strategy.



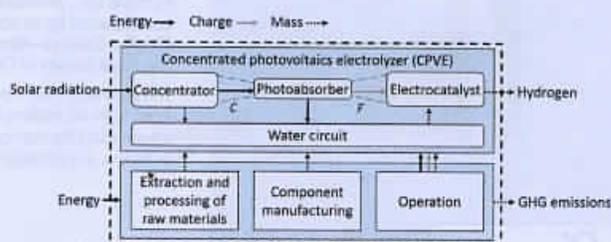
## ANALYSIS

3069

### Design guidelines for concentrated photo-electrochemical water splitting devices based on energy and greenhouse gas yield ratios

Mikaël Dumortier and Sophia Haussener\*

Solar irradiation concentration is considered a viable strategy for reducing the energy and financial investment of photo-electrochemical hydrogen generation.

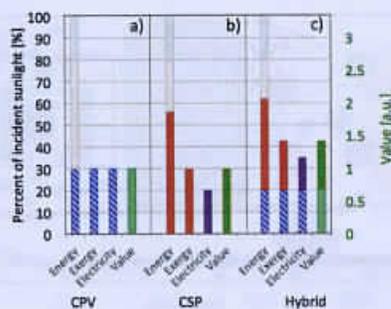


3083

### Hybrid solar converters for maximum exergy and inexpensive dispatchable electricity

Howard M. Branz,\* William Regan, Kacy J. Gerst, J. Brian Borak and Elizabeth A. Santori

Hybrid converters could optimally exploit the solar spectrum to realize higher conversion efficiencies and low electricity costs, while ensuring the availability of inexpensive dispatchable solar power.



## REVIEWS

3092

### Two-dimensional covalent carbon nitride nanosheets: synthesis, functionalization, and applications

Jinshui Zhang, Yan Chen and Xinchun Wang\*

This review presents a summary of the recent progress in synthesis, functionalization and application of two-dimensional covalent carbon nitride nanosheets.



3109

### Application of computational chemistry in understanding the mechanisms of mercury removal technologies: a review

Lixia Ling, Maohong Fan,\* Baojun Wang\* and Riguan Zhang

Computational chemistry is a useful method to understand the mechanisms of mercury removal.

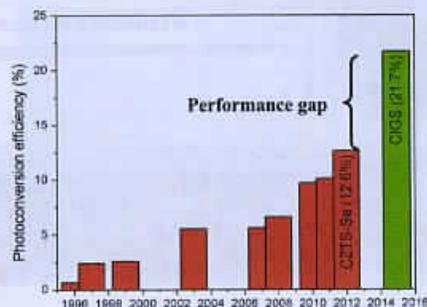


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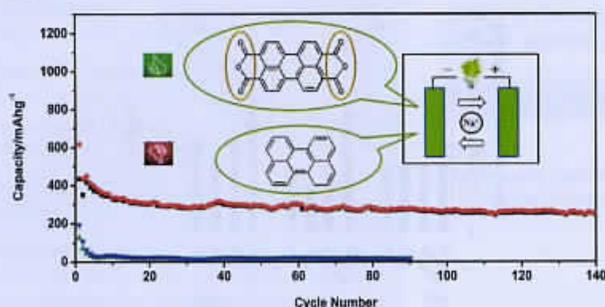
### Strategic review of secondary phases, defects and defect-complexes in kesterite CZTS–Se solar cells

Mukesh Kumar,\* Ashish Dubey, Nirmal Adhikari, Swaminathan Venkatesan and Qiquan Qiao\*

This article presents a strategic review of secondary phases, defects and defect-complexes in kesterite CZTS–Se solar cells responsible for performance gap from CIGS solar cells.



3160

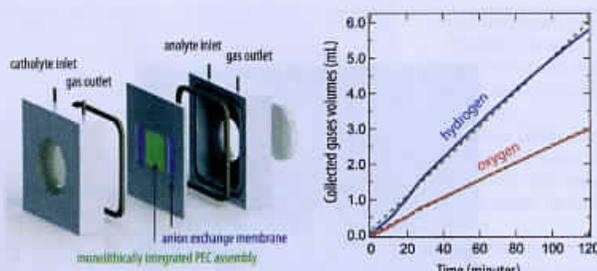


### Multi-ring aromatic carbonyl compounds enabling high capacity and stable performance of sodium-organic batteries

Heng-guo Wang, Shuang Yuan, Zhenjun Si and Xin-bo Zhang\*

Herein we report that organic compounds comprising planar  $C_6$  ring structures and carboxylate groups can function as an excellent anode material for sodium-organic batteries.

3166

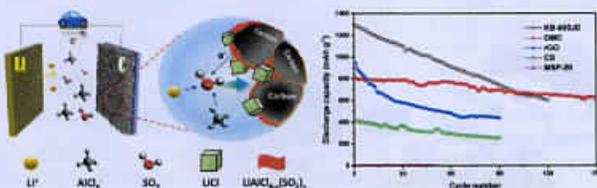


### A monolithically integrated, intrinsically safe, 10% efficient, solar-driven water-splitting system based on active, stable earth-abundant electrocatalysts in conjunction with tandem III-V light absorbers protected by amorphous $TiO_2$ films

Erik Verlage, Shu Hu, Rui Liu, Ryan J. R. Jones, Ke Sun, Chengxiang Xiang,\* Nathan S. Lewis\* and Harry A. Atwater\*

A monolithically integrated device, protected by a  $TiO_2$  stabilization layer, splits water using sunlight.

3173

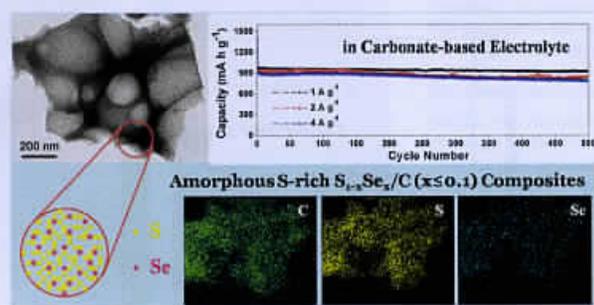


### Nanotechnology enabled rechargeable Li-SO<sub>2</sub> batteries: another approach towards post-lithium-ion battery systems

Goojin Jeong, Hansu Kim,\* Jong Hwan Park, Jaehwan Jeon, Xing Jin, Juhye Song, Bo-Ram Kim, Min-Sik Park, Ji Man Kim\* and Young-Jun Kim\*

Recent achievements in the nanotechnology show the full potential of Li-SO<sub>2</sub> rechargeable batteries to be regarded as an alternative to the currently used LIBs.

3181



### Amorphous S-rich $S_{1-x}Se_x/C$ ( $x \leq 0.1$ ) composites promise better lithium-sulfur batteries in a carbonate-based electrolyte

Xiaona Li, Jianwen Liang, Kailong Zhang, Zhiguo Hou, Wanqun Zhang, Yongchun Zhu\* and Yitai Qian\*

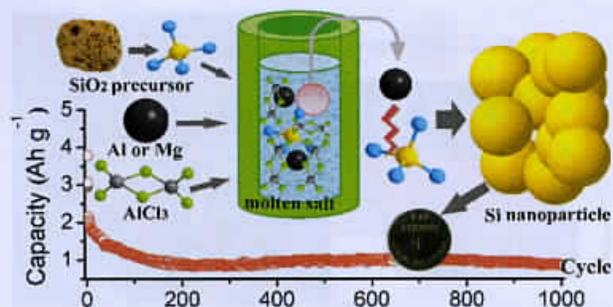
The low electrochemical utilization of S and fast capacity fading can be effectively diminished by immobilizing sulfur in porous carbon via the interaction of a small amount of selenium in S-rich  $S_{1-x}Se_x/C$  ( $x \leq 0.1$ ) composites.

3187

### A low temperature molten salt process for aluminothermic reduction of silicon oxides to crystalline Si for Li-ion batteries

Ning Lin, Ying Han, Jie Zhou, Kailong Zhang, Tianjun Xu, Yongchun Zhu\* and Yitai Qian\*

A molten salt system is developed for low-temperature metallothermic reduction of various silicates or silica to crystalline Si nanoparticles as high-performance anode materials.



3192

### Dithienopicenocarbazole as the kernel module of low-energy-gap organic dyes for efficient conversion of sunlight to electricity

Zhaoyang Yao, Heng Wu, Yang Li, Junting Wang, Jing Zhang, Min Zhang,\* Yanchun Guo and Peng Wang\*

A metal-free organic dye-sensitized solar cell attains 13% power conversion efficiency under AM1.5G full sunlight.

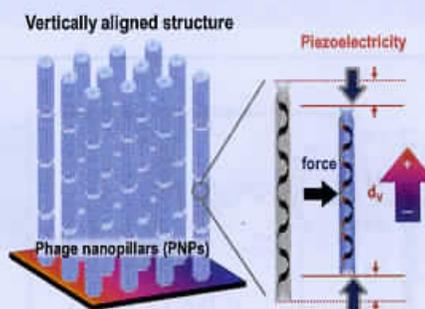


3198

### Bioinspired piezoelectric nanogenerators based on vertically aligned phage nanopillars

Dong-Myeong Shin, Hye Ji Han, Won-Geun Kim, Eunjong Kim, Chuntae Kim, Suck Won Hong, Hyung Kook Kim, Jin-Woo Oh\* and Yoon-Hwae Hwang\*

Bioinspired piezoelectric nanogenerators based on phage nanopillars are ineptively demonstrated, and the electrical power from phage nanopillars holds promise for the development of implantable and wearable electronics.

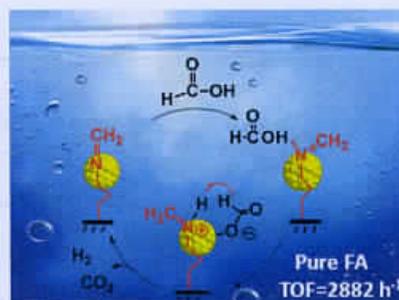


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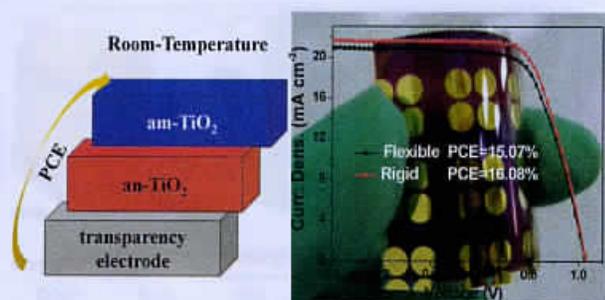
### A Schiff base modified gold catalyst for green and efficient H<sub>2</sub> production from formic acid

Qinggang Liu, Xiaofeng Yang, Yanqiang Huang,\* Shutao Xu, Xiong Su, Xiaoli Pan, Jinming Xu, Aiqin Wang, Changhai Liang, Xinkui Wang\* and Tao Zhang\*

A novel Schiff base modified gold nanocatalyst was designed for H<sub>2</sub> production from pure formic acid (FA) without any additives.



3208

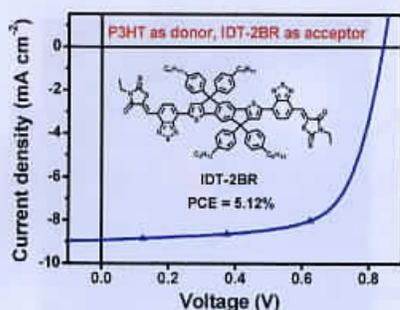


### High efficiency flexible perovskite solar cells using superior low temperature TiO<sub>2</sub>

Dong Yang, Ruixia Yang, Jing Zhang, Zhou Yang, Shengzhong (Frank) Liu\* and Can Li\*

15.07% efficiency for flexible perovskite solar cells is achieved using low temperature TiO<sub>2</sub>.

3215



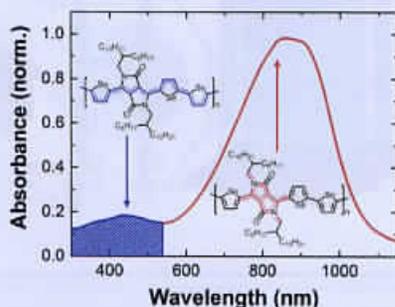
### A planar electron acceptor for efficient polymer solar cells

Yao Wu, Huitao Bai, Zaiyu Wang, Pei Cheng, Siya Zhu, Yifan Wang, Wei Ma and Xiaowei Zhan\*

Polymer solar cells (PSCs) based on blended films of a novel planar acceptor and P3HT gave power conversion efficiencies of up to 5.12%, which are much higher than that of PC<sub>61</sub>BM-based control devices (3.71%) and the highest values reported for P3HT-based fullerene-free PSCs.

## PAPERS

3222

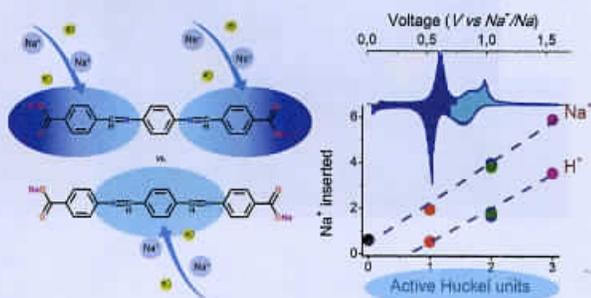


### Natures of optical absorption transitions and excitation energy dependent photostability of diketopyrrolopyrrole (DPP)-based photovoltaic copolymers

Sebastian Wood, Jessica Wade, Munazza Shahid, Elisa Collado-Fregoso, Donal D. C. Bradley, James R. Durrant, Martin Heeney and Ji-Seon Kim\*

The photostability of diketopyrrolopyrrole (DPP)-based copolymers is examined by investigating the natures of the two dominant optical absorption transitions.

3233



### Oligomeric-Schiff bases as negative electrodes for sodium ion batteries: unveiling the nature of their active redox centers

María López-Herraz, Elizabeth Castillo-Martinez,\* Javier Carretero-González, Javier Carrasco, Teófilo Rojo and Michel Armand\*

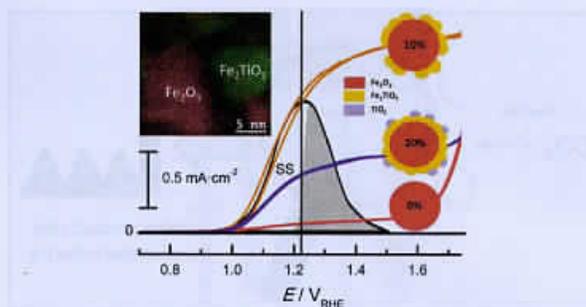
Novel hybrids between carboxylate and aromatic Schiff base show reversible sodium insertion below 1.2 V vs. Na<sup>+</sup>. Identifying the redox active units leads to sustainable and low cost anode materials beyond 250 mA h g<sup>-1</sup>.

3242

### What do you do, titanium? Insight into the role of titanium oxide as a water oxidation promoter in hematite-based photoanodes

Damián Monllor-Satoca,\* Mario Bärtsch, Cristian Fàbrega, Aziz Genç, Sandra Reinhard, Teresa Andreu,\* Jordi Arbiol, Markus Niederberger and Joan Ramon Morante

Titanium improves water oxidation yields over hematite photoanodes, tailoring its surface state density (kinetics) and hematite-pseudobrookite heterojunctions (energetics).

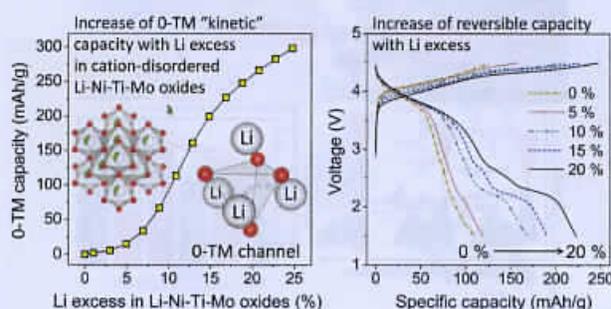


3255

### A new class of high capacity cation-disordered oxides for rechargeable lithium batteries: Li-Ni-Ti-Mo oxides

Jinhyuk Lee, Dong-Hwa Seo, Mahalingam Balasubramanian, Nancy Twu, Xin Li and Gerbrand Ceder\*

Percolation theory enables the design of high capacity cation-disordered oxides for rechargeable lithium battery cathodes.

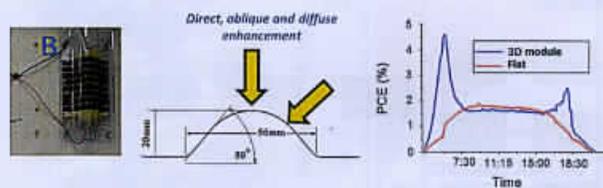


3266

### Three dimensional corrugated organic photovoltaics for building integration; improving the efficiency, oblique angle and diffuse performance of solar cells

Jeff Kettle,\* Noel Bristow, Tracy K. N. Sweet, Nick Jenkins, Gisele A. dos Reis Benatto, Mikkel Jørgensen and Frederik C. Krebs

The lamination of OPV modules to corrugated roof cladding has been undertaken.

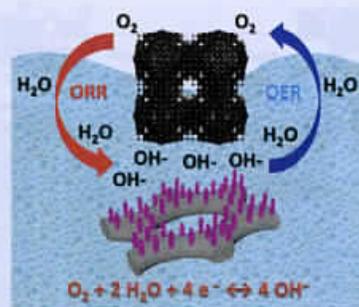


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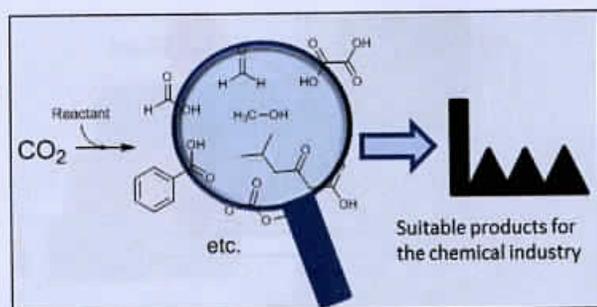
### Hierarchical pore-in-pore and wire-in-wire catalysts for rechargeable Zn- and Li-air batteries with ultra-long cycle life and high cell efficiency

Longjun Li, Chao Liu, Guang He, Donglei Fan and Arumugam Manthiram\*

Inexpensive hierarchical oxygen reduction and oxygen evolution reaction (ORR/OER) catalysts offer higher cell efficiency and much longer cycle life than Pt/C + IrO<sub>2</sub> bifunctional catalysts in metal-air batteries.



3283

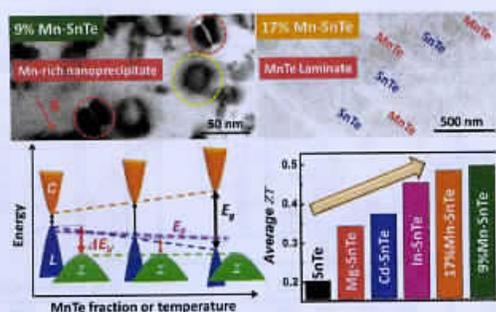


### Closing the loop: captured $\text{CO}_2$ as a feedstock in the chemical industry

Alexander Otto,\* Thomas Grube, Sebastian Schiebahn and Detlef Stolten

Identification of  $\text{CO}_2$  utilization reactions that have the most potential for future technical exploration and implementation within the chemical industry.

3298

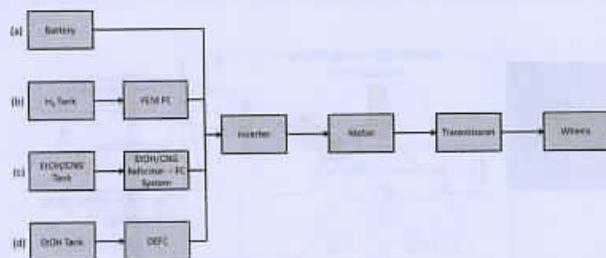


### Synergistically optimized electrical and thermal transport properties of SnTe via alloying high-solubility MnTe

Haijun Wu, Cheng Chang, Dan Feng, Yu Xiao, Xiao Zhang, Yanling Pei, Lei Zheng, Di Wu, Shengkai Gong, Yue Chen, Jiaqing He,\* Mercuri G. Kanatzidis\* and Li-Dong Zhao\*

Heavy MnTe alloying can significantly improve the electrical and thermal transport properties of SnTe via multiple approaches.

3313

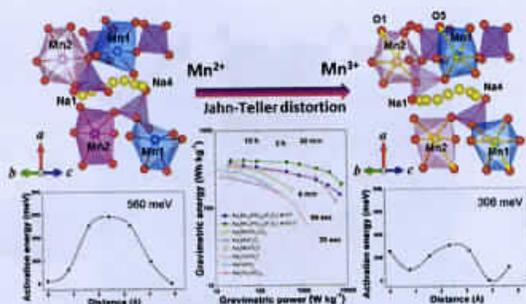


### Well to wheel analysis of low carbon alternatives for road traffic

Srikanth Ramachandran and Ulrich Stimming\*

A FCEV based on bio-ethanol derived from organic waste can be a more sustainable alternative to BEVs and  $\text{H}_2$ -FCEVs.

3325



### Anomalous Jahn–Teller behavior in a manganese-based mixed-phosphate cathode for sodium ion batteries

Hyungsub Kim, Gabin Yoon, Inchul Park, Kyu-Young Park, Byungju Lee, Jongsoo Kim, Young-Uk Park, Sung-Kyun Jung, Hee-Dae Lim, Docheon Ahn, Seongsu Lee and Kisuk Kang\*

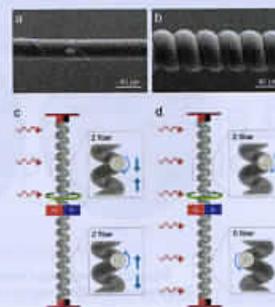
We report a 3.8 V manganese-based mixed-phosphate cathode material for applications in sodium rechargeable batteries; *i.e.*,  $\text{Na}_4\text{Mn}_3(\text{PO}_4)_2(\text{P}_2\text{O}_7)$ .

3336

### Harvesting temperature fluctuations as electrical energy using torsional and tensile polymer muscles

Shi Hyeong Kim, Márcio D. Lima, Mikhail E. Kozlov, Carter S. Haines, Geoffrey M. Spinks, Shazed Aziz, Changsoon Choi, Hyeon Jun Sim, Xuemin Wang, Hongbing Lu, Dong Qian, John D. W. Madden, Ray H. Baughman\* and Seon Jeong Kim\*

Low-grade waste heat is harvested as electrical energy by employing thermally-powered torsional and tensile artificial muscles made from inexpensive polymer fibers used for fishing line and sewing thread.

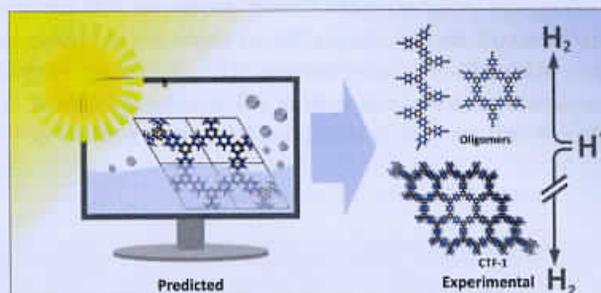


3345

### Phenyl-triazine oligomers for light-driven hydrogen evolution

K. Schwinghammer, S. Hug, M. B. Mesch, J. Senker and B. V. Lotsch\*

Carbon nitride oligomers derived from the covalent triazine framework CTF-1 constitute a new generation of tunable hydrogen evolution photocatalysts, which show moderate activities even without the addition of a co-catalyst.

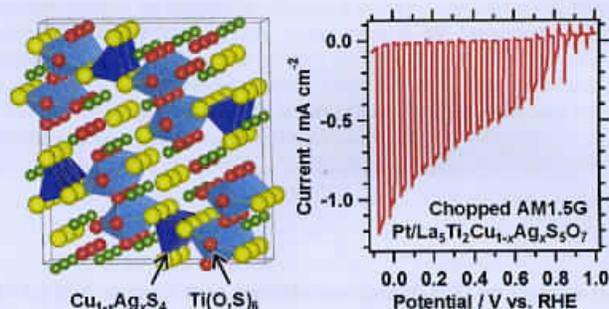


3354

### La<sub>5</sub>Ti<sub>2</sub>Cu<sub>1-x</sub>Ag<sub>x</sub>S<sub>5</sub>O<sub>7</sub> photocathodes operating at positive potentials during photoelectrochemical hydrogen evolution under irradiation of up to 710 nm

Takashi Hisatomi, Shintaro Okamura, Jingyuan Liu, Yuki Shinohara, Koichiro Ueda, Tomohiro Higashi, Masao Katayama, Tsutomu Minegishi and Kazunari Domen\*

Photoelectrodes of Al-doped La<sub>5</sub>Ti<sub>2</sub>Cu<sub>1-x</sub>Ag<sub>x</sub>S<sub>5</sub>O<sub>7</sub> powder generate a photocathodic current attributable to the hydrogen evolution reaction at +0.7 V vs. RHE.

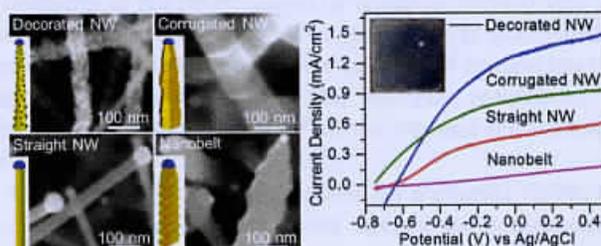


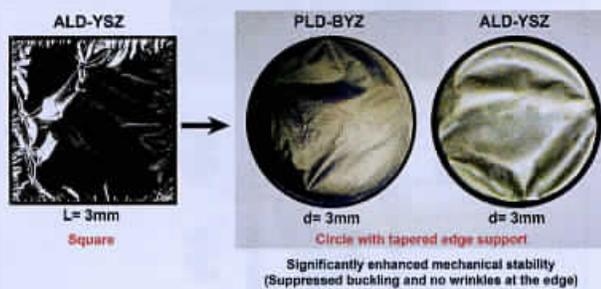
3363

### Defect-rich decorated TiO<sub>2</sub> nanowires for super-efficient photoelectrochemical water splitting driven by visible light

Md Anisur Rahman, Samad Bazargan, Saurabh Srivastava, Xiongyao Wang, Marwa Abd-Ellah, Joseph P. Thomas, Nina F. Heinig, Debabrata Pradhan and Kam Tong Leung\*

Defect-rich 1D TiO<sub>2</sub> nanostructures show excellent photoelectrochemical water splitting property in the visible light region with a low onset potential of 0.3 V vs. RHE and a remarkably high conversion efficiency of 3.6%.





## A circular membrane for nano thin film micro solid oxide fuel cells with enhanced mechanical stability

Jong Dae Baek, Yong-Jin Yoon, Wonyoung Lee and Pei-Chen Su\*

We demonstrate a new architecture for a low temperature solid oxide fuel cell to enlarge the lateral dimension of the fragile nano thin film electrolyte from the micrometer to millimeter scale with greatly enhanced mechanical stability.

