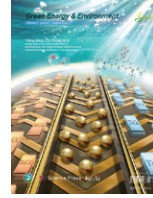




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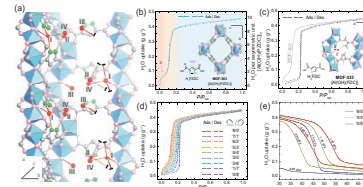
## CONTENTS

### Research highlight

**Multivariate MOF for optimizing atmospheric water harvesting**

Ao Ma, Hengjiang Cong\*, Hexiang Deng..... 575

Atmospheric water harvesting offers a powerful and promising solution to address the problem of global freshwater scarcity. In the past decade, significant progress has been achieved in utilizing hydrolytically stable metaleorganic frameworks as recyclable water-sorbent materials under low relative humidity, especially in those arid areas. Recently, Yaghi's group has employed a combined crystallographic and theoretical technique to decipher the water filling mechanism in MOF-303, where the polar organic linkers rather than the inorganic units of MOF are demonstrated as the key factor. Hence, the hydrophilic strength of the water-binding pocket in MOFs can be optimized through the approach of multivariate modulations, resulting in enhanced water harvesting properties.

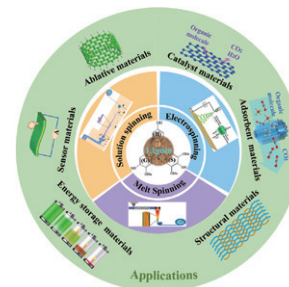


### Review articles

**Lignin-based carbon fibers: Formation, modification and potential applications**

Shichao Wang\*, Jixing Bai, Mugaanire Tendo Innocent, Qianqian Wang, Hengxue Xiang\*, Jianguo Tang\*, Meifang Zhu..... 578

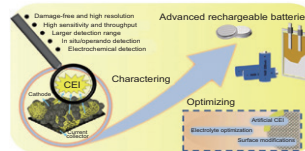
Formation, modification and potential applications of lignin-based carbon fibers were deeply discussed based on the relationships among chemical structure, processing conditions and Suggestions for further development of lignin-based carbon fibers were also proposed.



**Charactering and optimizing cathode electrolytes interface for advanced rechargeable batteries: Promises and challenges**

Zhongyang Zhang, Xinran Wang\*, Ying Bai, Chuan Wu\*..... 606

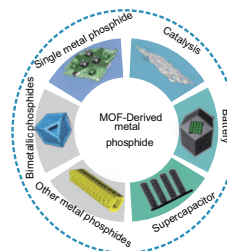
In order to promote the benign development of battery field, we put forward the idea from characterization to optimization in view of the challenges faced by the research of the CEI.



## Metal-organic frameworks-derived metal phosphides for electrochemistry application

Xinru Tang, Nan Li, Huan Pang\* ..... 636

In this review, we discuss the classification of MOF-derived metal phosphides materials, and introduce their applications in the field of electrochemistry, including catalysis, batteries and supercapacitors.

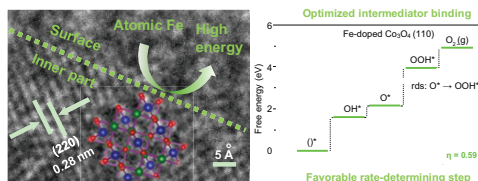


## Research papers

### Surface-mediated iron on porous cobalt oxide with high energy state for efficient water oxidation electrocatalysis

Jingsha Li, Tao Hu, Changhong Wang, Chunxian Guo\* ..... 662

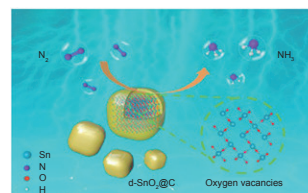
A surface-mediated incorporation strategy is designed to realize desired energy state and coordination environment for spinel  $\text{Co}_3\text{O}_4$ , enabling optimized intermediate binding and favorably changing the rate-determining step for enhanced oxygen evolution electrocatalysis.



### Oxygen-deficient $\text{SnO}_2$ nanoparticles with ultrathin carbon shell for efficient electrocatalytic $\text{N}_2$ reduction

Guangkai Li<sup>1</sup>, Haeseong Jang<sup>1</sup>, Zijian Li, Jia Wang, Xuqiang Ji\*, Min Gyu Kim, Xien Liu\*, Jaephil Cho\* ..... 672

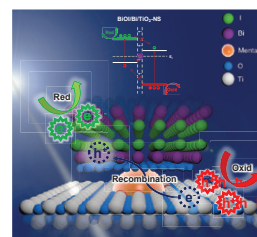
Oxygen-deficient  $\text{SnO}_2$  nanoparticles with ultrathin carbon shell are constructed for  $\text{N}_2$ -to- $\text{NH}_3$  catalysis with  $\text{NH}_3$  Faradic efficiency as high as 12.7% at -0.15 V vs. RHE in 0.1 mol  $\text{L}^{-1}$  HCl.



### Design and in-situ construct BiOI/Bi/TiO<sub>2</sub> photocatalysts with metal-mediated heterostructures employing oxygen vacancies in TiO<sub>2</sub> nanosheets

Chenchen Zhang, Wenbin Chen, Dairong Hu, Hanjie Xie, Yibing Song\*, Binbin Luo, Yiwen Fang, Wenhua Gao, Ziyi Zhong\* ..... 680

The BiOI/Bi/TiO<sub>2</sub>-NS photocatalyst possesses the merits of the p-n junction for energy band manipulating, and that of the Z-scheme photocatalyst for photogenerated charge carrier separation and high redox capability, thus exhibiting much improved photocatalytic performance.



## Vicinal hydroxyl group-inspired selective oxidation of glycerol to glyceric acid on hydroxyapatite supported Pd catalyst

Difan Li, Xiuge Zhao, Qingqing Zhou, Bingjie Ding, Anna Zheng, Qingpo Peng, Zhenshan Hou\*.....

691

The hydroxyapatite-supported Pd has been used as a bi-functional catalyst and exhibited excellent performance for selective oxidation of vicinal diol to  $\alpha$ -hydroxycarboxylic acid with molecular oxygen as terminal oxidant under mild conditions.

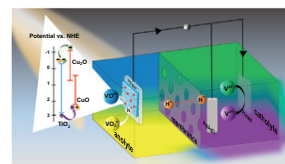


## High performance of TiO<sub>2</sub>/Cu<sub>x</sub>O photoelectrodes for regenerative solar energy storage in a vanadium photoelectrochemical cell

Harin Yoo, Doohwan Lee, Jung Hyeun Kim\*.....

704

Vanadium redox electrolyte pairs are used in the anode and cathode chambers for efficient charge transfers through the z-scheme assisted potential energy distributions in the TiO<sub>2</sub>/Cu<sub>x</sub>O photoanode film.

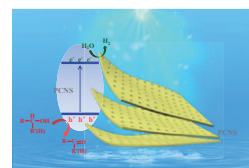


## Visible light-driven oxidant-free dehydrogenation of alcohols in water using porous ultrathin g-C<sub>3</sub>N<sub>4</sub> nanosheets

Wei Zhang<sup>1</sup>, Jiajun Wang<sup>1</sup>, Zewei Liu, Yibing Pi, Rong Tan\*.....

712

Porous ultrathin g-C<sub>3</sub>N<sub>4</sub> nanosheets enabled oxidant-free dehydrogenation of alcohols to be efficiently performed in water, by using visible light as the sole energy input.

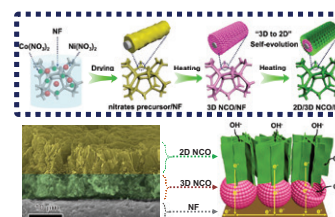


## High mass loading NiCo<sub>2</sub>O<sub>4</sub> with shell-nanosheet/core-nanocage hierarchical structure for high-rate solid-state hybrid supercapacitors

Wang Yang<sup>1</sup>, Liqiang Hou<sup>1</sup>, Peng Wang, Yun Li, Rui Li, Bo Jiang, Fan Yang, Yongfeng Li\*.....

723

A hierarchical NiCo<sub>2</sub>O<sub>4</sub> structure with nanosheets-shell and nanocages-core is directly grown on nickel foam through a 3D-to-2D self-evolution process, and the as-prepared free-standing electrode with ultrahigh mass loading delivers an excellent capacity, high-rate capability, and robust cycle stability for supercapacitors.

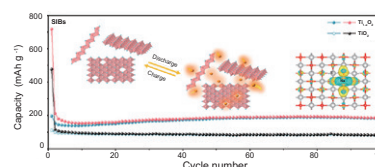


## Engineering electronic structures of titanium vacancies in Ti<sub>1-x</sub>O<sub>2</sub> nanosheets enables enhanced Li-ion and Na-ion storage

Huiqin Wang, Fengchu Zhang, Jing Xia, Fei Lu, Bo Zhou, Ding Yi, Xi Wang\*.....

734

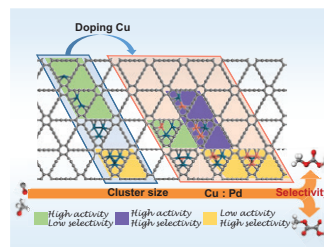
The Ti<sub>1-x</sub>O<sub>2</sub> nanosheets exhibit higher electrochemical properties than stoichiometric TiO<sub>2</sub> nanosheets via employing the electronic structures of Ti vacancies. Therefore, for the Ti<sub>1-x</sub>O<sub>2</sub>, in addition to a redox intercalation process, extra Li-ion and Na-ion are adsorbed on the Ti vacancies.



## The regulating effect of doping Cu on the catalytic performance of CO oxidative coupling to DMO on Pd<sub>x</sub>Cu<sub>y</sub>/GDY: A DFT study

Juan Zhao, Min Han, Zhanhui Wang, Lixia Ling\*, Riguang Zhang, Baojun Wang\*..... 742

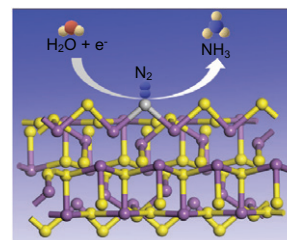
The catalytic performance of Pd<sub>x</sub>/GDY (x = 1, 2, 3, 4) aiming at CO oxidative coupling reaction is poor, and then doping the second metal Cu to adjust the catalytic performance. Pd<sub>1</sub>Cu<sub>1</sub>/GDY and Pd<sub>1</sub>Cu<sub>2</sub>/GDY exhibit high catalytic acidity and selectivity to DMO.



## Sulfur vacancies-doped Sb<sub>2</sub>S<sub>3</sub> nanorods as high-Efficient electrocatalysts for dinitrogen fixation under ambient conditions

Xuyan Wang, Jianwei Bai, Yantao Wang, Xiaoying Lu, Zehua Zou, Junfeng Huang, Cailing Xu\*..... 755

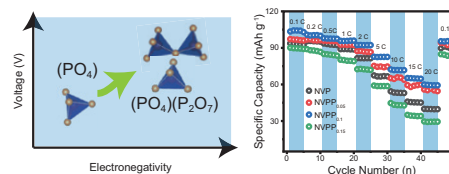
This work successfully performs defect engineering by hydrogenation process. The as-constructed sulfur vacancies-doped Sb<sub>2</sub>S<sub>3</sub> nanorods (Sv-Sb<sub>2</sub>S<sub>3</sub>) exhibits boosted electrocatalytic N<sub>2</sub> reduction (NRR) performance compared to bulk material.



## Enhanced electrode kinetics and properties via anionic regulation in polyanionic Na<sub>3+x</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3-x</sub>(P<sub>2</sub>O<sub>7</sub>)<sub>x</sub> cathode material

Mei-Yi Wang<sup>1</sup>, Xin-Xin Zhao<sup>1</sup>, Jin-Zhi Guo, Xue-Jiao Nie, Zhen-Yi Gu, Xu Yang, Xing-Long Wu\*... 763

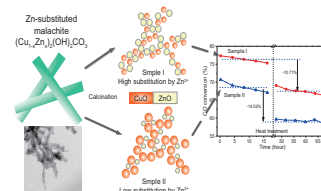
Anion-site regulation by substituting P<sub>2</sub>O<sub>7</sub><sup>4-</sup> to PO<sub>4</sub><sup>3-</sup> is achieved to prepare Na<sub>3+x</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3-x</sub>(P<sub>2</sub>O<sub>7</sub>)<sub>x</sub> cathode materials, which improved working voltage and electrochemical properties. In addition, the theoretical and experimental analyses reveal the anionic manipulation mechanism of the P<sub>2</sub>O<sub>7</sub><sup>4-</sup>.



## Improved methanol synthesis performance of Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst by controlling its precursor structure

Fan Zhang\*, Xiaoying Xu, Zhenpu Qiu, Bo Feng, Yuan Liu, Aihua Xing, Maohong Fan\*..... 772

Fractional precipitation promoted zinc substitution in the malachite lattice. Derived from highly zinc-substituted malachite, sample I demonstrated better catalytic activity and thermostability during the methanol synthesis reaction from syngas.

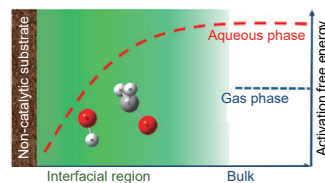


## A reaction density functional theory study of solvent effect in the nucleophilic addition reactions in aqueous solution

Cheng Cai, Weiqiang Tang, Chongzhi Qiao, Bo Bao, Peng Xie\*, Shuangliang Zhao\*, Honglai Liu\*..... 782

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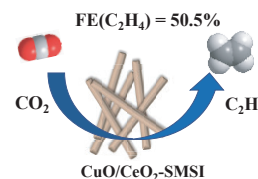
When the reaction core of the  $\text{OH}^- + \text{HCHO}$  reaction is closed to the graphene-like wall, the activation free energy is lower than the barrier energy in bulk aqueous solution, but it recovers to the bulk value when the reaction core is far away from the wall.



## Enhanced $\text{CO}_2$ electroreduction to ethylene via strong metal-support interaction

Mengen Chu, Chunjun Chen, Yahui Wu, Xupeng Yan, Shuaiqiang Jia, Ruting Feng, Haihong Wu\*, Mingyuan He\*, Buxing Han\*..... 792

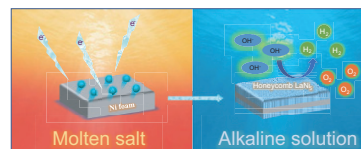
The  $\text{CuO}/\text{CeO}_2$ -SMSI with strong metal-support interaction could efficiently electroreduction of  $\text{CO}_2$  to  $\text{C}_2\text{H}_4$ . The strong metal-support interaction could not only enhance the adsorption and activation of  $\text{CO}_2$ , but also can stabilize the  $\text{CuO}$ .



## Hierarchical and self-supporting honeycomb $\text{LaNi}_5$ alloy on nickel foam for overall water splitting in alkaline media

Yanze Wu, Yalan Liu, Kui Liu, Lin Wang, Lei Zhang, Degao Wang, Zhifang Chai, Weiqun Shi\*..... 799

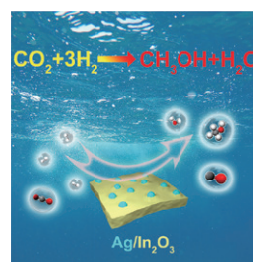
Hierarchical honeycomb  $\text{LaNi}_5$  alloy on Ni foam was obtained by depositing high reactive element La directly on Ni foam in molten salt, which could simultaneously realize hydrogen evolution reaction and oxygen evolution reaction efficiently.



## The feasibility study of the indium oxide supported silver catalyst for selective hydrogenation of $\text{CO}_2$ to methanol

Kaihang Sun, Zhitao Zhang, Chenyang Shen, Ning Rui, Chang-jun Liu\*..... 807

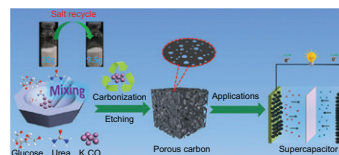
The feasibility of selective hydrogenation of carbon dioxide to methanol on  $\text{Ag}/\text{In}_2\text{O}_3$  has been confirmed theoretically and experimentally. The intense  $\text{Ag}-\text{In}_2\text{O}_3$  interaction promotes the formation of oxygen vacancy, causing the enhanced activation and dissociation of  $\text{CO}_2$ . The enhanced  $\text{CO}_2$  dissociation leads to the methanol synthesis via the  $\text{CO}$  hydrogenation route.



## One-pot green mass production of hierarchically porous carbon via a recyclable salt-templating strategy

Changde Ma, Jiang Gong, Shuang Zhao, Xiaoguang Liu, Xueying Mu, Yanhui Wang\*, Xuecheng Chen\*, Tao Tang\*..... 818

Hierarchically porous carbon has been prepared via a recyclable salt-templating strategy, and the prepared porous carbon exhibited excellent electrochemical performance when used as electrode material in supercapacitors.

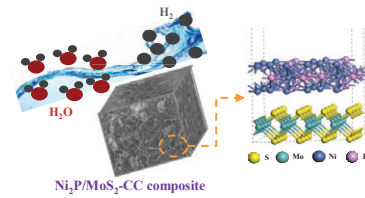


## $\text{Ni}_2\text{P}/\text{MoS}_2$ interfacial structures loading on N-doped carbon matrix for highly efficient hydrogen evolution

Yuelong Xu<sup>1</sup>, Ran Wang<sup>1</sup>, Zhan Liu, Lili Gao, Tifeng Jiao\*, Zhenfa Liu\*..... 829



The N-doped porous carbon matrix loaded with Ni<sub>2</sub>P/MoS<sub>2</sub> was prepared through a simple hydrothermal-phosphorization method. The synergetic interfacial effect between Ni<sub>2</sub>P and MoS<sub>2</sub> provided good electrocatalytic performance and high stability for hydrogen evolution.



## Increasing the greenness of an organic acid through deep eutectic solvation and further polymerization

Liteng Li, Xiaofang Li, Susu Zhang, Hongyuan Yan, Xiaoqiang Qiao, Hongyan He\*, Tao Zhu\*, Baokun Tang\*.....

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The toxicity of acrylic acid as an important industrial chemical can be decreased through deep eutectic solvation and further polymerisation.

