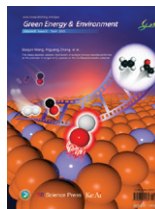




### Front Cover

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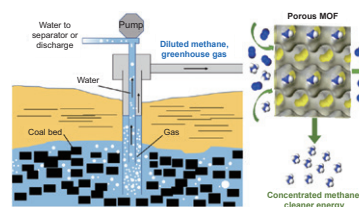
## CONTENTS

### Research highlight

#### Recovery of greenhouse gas as cleaner fossil fuel contributes to carbon neutrality

Xing Zhang, Jian-Rong Li\* ..... 351

This work highlights a recent publication by Yang *et al.* regarding to low concentration methane capture from coal bed methane using MOF sorbents. Such technology is promising to reduce greenhouse gas emission and promote the methane production capability, which would contribute to carbon neutrality in dual pathways.

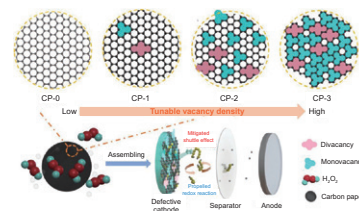


### Short communication

#### Tunable vacancy defect chemistry on free-standing carbon cathode for lithium-sulfur batteries

Xi Zhang, Xiaohong Liu, Wei Zhang\*, Yingze Song\* ..... 354

The defect engineering-enabled carbon cathode realizes not only the synergy of monovacancies and divacancies but also the tailor of defect density, leading to 3D electrocatalytic networks for Li-S redox reactions.

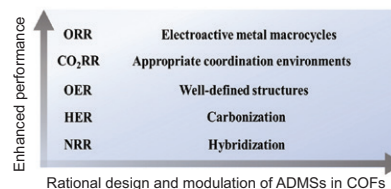


### Review articles

#### Atomically dispersed metal sites in COF-based nanomaterials for electrochemical energy conversion

Yaqi Cao, Wenchao Peng, Yang Li, Fengbao Zhang, Yuanzhi Zhu\*, Xiaobin Fan\* ..... 360

The recent progresses on the synthesis and electrochemical applications of atomically dispersed metal sites (ADMSs) in covalent organic frameworks (COFs) are summarized. Rational modulation strategies for enhanced electrocatalytic performance are highlighted, together with a discussion of the challenges and prospects.



# Green Energy & Environment

## Radical and (photo)electron transfer induced mechanisms for lignin photo- and electro-catalytic depolymerization

Kejia Wu<sup>1</sup>, Minglong Cao<sup>1</sup>, Qiang Zeng\*, Xuehui Li\* ..... 383

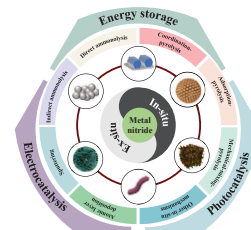
This review focus on radicals and (photo)electron transfers induced reaction mechanisms of photo(electro)catalytic lignin depolymerization and positive expects the prospect of photoelectrocatalysis(PEC) in lignin valorization.



## A review on the synthesis of transition metal nitride nanostructures and their energy related applications

Qiao Luo, Congcong Lu, Lingran Liu, Maiyong Zhu\* ..... 406

This review summarized the synthetic approaches toward metal nitride nanostructures by categorizing these methods into in-situ and ex-situ ones and presented their energy-related applications including energy storage, electrocatalysis and photocatalysis.

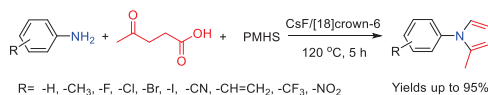


## Research papers

### Selectively reductive amination of levulinic acid with aryl amines to N-substituted aryl pyrroles

Cailing Wu, Mengjie Lou, Mingming Sun, Huiyong Wang, Zhiyong Li, Jikuan Qiu, Jianji Wang\*, Zhimin Liu\* ..... 438

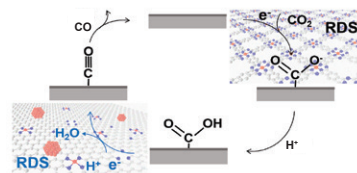
N-substituted aryl pyrroles can be produced via selectively reductive amination/cyclization of levulinic acid with aromatic amines and hydrosilane over CsF, with yields up to 95%.



### Phthalocyanine-derived catalysts decorated by metallic nanoclusters for enhanced CO<sub>2</sub> electroreduction

Jiacheng Chen, Jiayu Li, Jing Xu, Minghui Zhu\*, Yi-Fan Han\* ..... 444

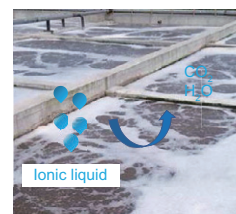
A catalyst containing Ni-N<sub>4</sub> and highly dispersed Ni<sup>0</sup> nanoclusters is reported. The electronic interaction between Ni-N<sub>4</sub> and Ni<sup>0</sup> increases the TOF<sub>CO</sub> by two folds and shifts the RDS of CO<sub>2</sub>RR.



### Complete degradation of high-loaded phenol using tungstate-based ionic liquids with long chain substituent at mild conditions

Yingying Yang, Honglei Fan\*, Tianbin Wu, Guanying Yang, Buxing Han\* ..... 452

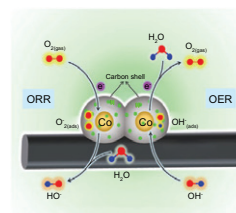
Tungstate-based ionic liquid ([Dodecyl(CH<sub>3</sub>)<sub>3</sub>N]<sub>2</sub>WO<sub>4</sub>) could degrade high-loaded phenol (48 g L<sup>-1</sup>) into gases and water completely at 323 K.



## Strengthening absorption ability of Co-N-C as efficient bifunctional oxygen catalyst by modulating the *d* band center using MoC

Jianwen Liu<sup>1</sup>, Ying Guo<sup>1</sup>, Xian-Zhu Fu, Jing-Li Luo\*, Chunyi Zhi\* ..... 459

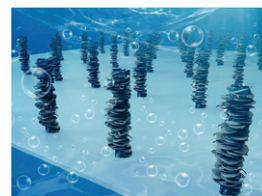
The bi-catalysts MoC/Co-N-C exhibits a high wave-half potential of 0.865 V for ORR and low overpotential of 370 mV for OER at 10 mA cm<sup>-2</sup>.



## Anchoring nitrogen-doped Co<sub>2</sub>P nanoflakes on NiCo<sub>2</sub>O<sub>4</sub> nanorod arrays over nickel foam as high-performance 3D electrode for alkaline hydrogen evolution

Xiaohao Ji, Xiaoyu Chen, Lijuan Zhang, Cheng Meng, Yilei He, Xing Zhang, Zumin Wang\*, Ranbo Yu\* ..... 470

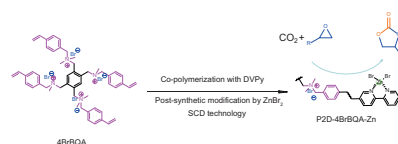
In this work, a practical 3D self-supported electrode was prepared. In this configuration, nitrogen doped Co<sub>2</sub>P nanoflakes were grown on NiCo<sub>2</sub>O<sub>4</sub> nanorod arrays supporting on nickel foam. Due to this novel hierarchal architecture, it possessed large active electrochemical active area, favorable wettability, increased ion transfer and reduced electronic resistance. Furthermore, by tuning the *d* band center through nitrogen doping, optimized hydrogen adsorption was achieved. Thus, N-Co<sub>2</sub>P/NiCo<sub>2</sub>O<sub>4</sub>/NF demonstrated superior activity and stability toward alkaline hydrogen evolution reaction.



## Mesoporous poly(ionic liquid)s with dual active sites for highly efficient CO<sub>2</sub> conversion

Yawen Fu, Yanan Xu, Zepeng Zeng, Abdul-Rauf Ibrahim, Jin Yang, Shuliang Yang, Yaqiang Xie, Yanzhen Hong, Yuzhong Su, Hongtao Wang, Yanliang Wang, Li Peng\*, Jun Li\*, Wendy L. Queen ... 478

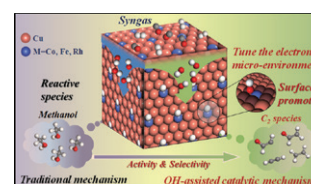
A novel mesoporous poly(ionic liquid) with dual active sites (nucleophilic and electrophilic sites) has been synthesized successfully, which offers excellent performance in CO<sub>2</sub> cycloaddition reaction under mild, solvent-free, and additive-free conditions.



## The newly-assisted catalytic mechanism of surface hydroxyl species performed as the promoter in syngas-to-C<sub>2</sub> species on the Cu-Based bimetallic catalysts

Chenyang Li<sup>1</sup>, Yuan Zhang<sup>1</sup>, Debao Li, Baojun Wang\*, Christopher K. Russell, Maohong Fan, Riguang Zhang\* ..... 487

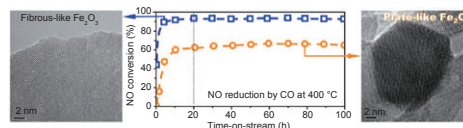
The function of surface OH is traditionally accepted as the hydrogenating reactive species in syngas conversion to C<sub>2</sub> species. This work for the first time proposed and confirmed the assisted catalytic mechanism of surface OH that performed as the promoter on Cu-based catalysts to promote the catalytic performance.



## Green rusts-derived iron oxide nanostructures catalyze NO reduction by CO

Ping Wang, Xiaoling Mou\*, Yong Li, Wenjie Shen..... 499

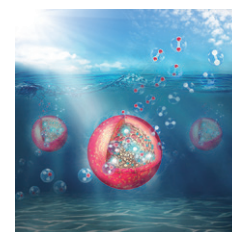
Fibrous-like and plate-like  $\alpha\text{-Fe}_2\text{O}_3$  nanocatalysts were synthesized by calcination of green rusts with different intercalating anions, showing distinct morphology effect in the NO reduction by CO reaction.



## A novel strategy for loading metal cocatalysts onto hollow nano-TiO<sub>2</sub> inner surface with highly enhanced H<sub>2</sub> production activity

Nan Chen, Yu Zhou, Songtao Cao, Ruixin Wang\*, Weizhou Jiao\*..... 509

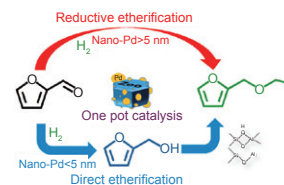
The in-situ pyrolysis of the predesigned complex of N-containing polymers and Pt at high temperature enhances the interaction between Pt and N-doped carbon (NC) layer. The resulted NC/Pt/TiO<sub>2</sub> hollow and porous photocatalyst shows the good conductivity, high charge transfer capacity and surface reaction activity, so as to provide excellent H<sub>2</sub> evolution efficiency.



## Efficient synthesis of bioetheric fuel additive by combining the reductive and direct etherification of furfural in one-pot over Pd nanoparticles deposited on zeolites

Xiaowen Guo, Haihong Wu, Peng Wu, Mingyuan He, Yejun Guan\*..... 519

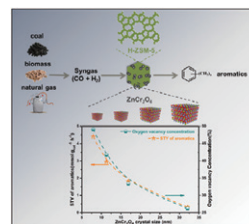
Spatially distributed Pd and acid sites on zeolites together contribute to the furfuryl ether ether production by catalyzing the reductive etherification and acid-catalyzed direct etherification in one-step.



## Insights into the size effect of ZnCr<sub>2</sub>O<sub>4</sub> spinel oxide in composite catalysts for conversion of syngas to aromatics

Yi Fu, Youming Ni, Wenhao Cui, Xudong Fang, Zhiyang Chen, Zhaopeng Liu, Wenliang Zhu\*, Zhongmin Liu\*..... 530

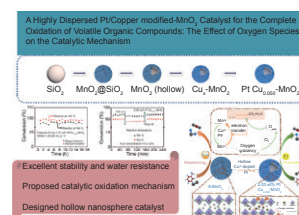
ZnCr<sub>2</sub>O<sub>4</sub> spinel oxide with a smaller size in ZnCr<sub>2</sub>O<sub>4</sub>&H-ZSM-5 composite catalyst possesses a higher oxygen vacancy concentration, which is conducive to enhance the space-time yield (STY) of aromatics in syngas to aromatics reaction.



## A highly dispersed Pt/copper modified-MnO<sub>2</sub> catalyst for the complete oxidation of volatile organic compounds: The effect of oxygen species on the catalytic mechanism

Xunxun Li, Yaru Wang, Dongyun Chen\*, Najun Li, Qingfeng Xu, Hua Li, Jinghui He, Jianmei Lu\*... 538

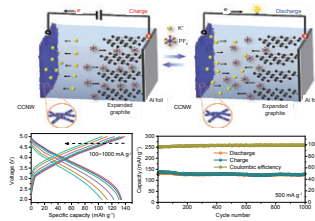
In this research, a series of  $y$  wt% Pt Cu<sub>0.050</sub>-MnO<sub>2</sub> catalysts were fabricated and their catalytic performance for toluene and benzene oxidation were investigated. We mainly focused on the relationship between oxygen species and catalytic performance.



## Coral-like and binder-free carbon nanowires for potassium dual-ion batteries with superior rate capability and long-term cycling life

Min Wang, Qirong Liu\*, Guangming Wu, Jianmin Ma, Yongbing Tang\* ..... 548

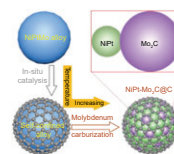
Coral-like carbon nanowires (CCNWs) doped with nitrogen as a binder-free anode were prepared for  $K^+$ -ion storage in dual-ion batteries, in which the unique coral-like porous nanostructure and amorphous/short-range-ordered composite feature are beneficial to enhance the structural stability, to facilitate the ion transfer and to boost the full utilization of active sites.



## Stable NiPt-Mo<sub>2</sub>C active site pairs enable boosted water splitting and direct methanol fuel cell

Jing Li, Zhu Guo, Wenjie Zhang, Jing Guo, Konggang Qu, Weiwei Cai\* ..... 559

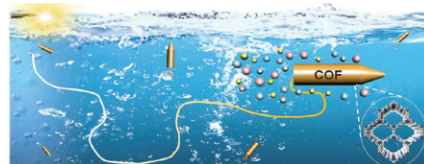
Stable NiPt-Mo<sub>2</sub>C active site pairs engineered *via* a self-confinement process can boost HER and MOR catalytic activity of Pt by 33 and 10.5 times, respectively.



## Visible light triggered exfoliation of COF micro/nanomotors for efficient photocatalysis

Kai Feng<sup>1</sup>, Liang Zhang<sup>1</sup>, Jiang Gong\*, Jinping Qu, Ran Niu\* ..... 567

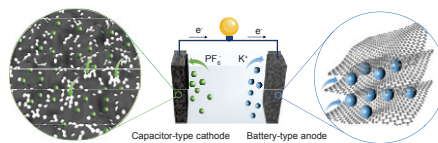
A new facile light-induced strategy based on diffusio-phoretic self-propulsion was proposed to disperse micron-sized aggregated bulk covalent organic frameworks (COFs) into nano-sized isolated COFs solutions for efficient degradation of organic pollutants.



## Nitrogen-doped porous carbon nanosheets as both anode and cathode for advanced potassium-ion hybrid capacitors

Quanzhou Du, Yuhua Zhao, Yujuan Chen, Jianming Liu, Huanhuan Li, Guangyue Bai, Kelei Zhuo\*, Jianji Wang\* ..... 579

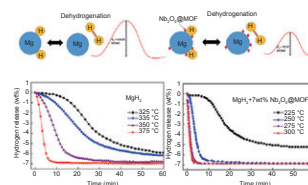
The prepared material owns the unique structure and exhibits remarkable potassium storage performance. Potassium-ion hybrid capacitors assembled by using the prepared material as both anode and cathode, which can alleviate the imbalance between reaction kinetics and specific capacity, deliver superior energy density.



## Metal organic framework supported niobium pentoxide nanoparticles with exceptional catalytic effect on hydrogen storage behavior of MgH<sub>2</sub>

Liuting Zhang\*, Farai Michael Nyahuma, Haoyu Zhang, Changshan Cheng, Jiaguang Zheng, Fuying Wu, Lixin Chen ..... 589

The uniformly distributed Nb<sub>2</sub>O<sub>5</sub> and MOF synergistically enhanced the dehydrogenation performance of MgH<sub>2</sub>.

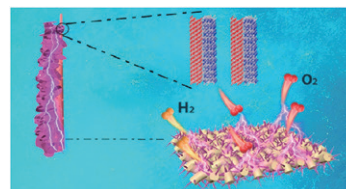




## Vacancies and interfaces engineering of core-shell heterostructured NiCoP/NiO as trifunctional electrocatalysts for overall water splitting and zinc-air batteries

Xiaolin Hu<sup>1</sup>, Jichuan Fan<sup>1</sup>, Ronghua Wang\*, Meng Li, Shikuan Sun, Chaohe Xu\*, Fusheng Pan ..... 601

Oxygen vacancies dominated porous NiCoP/NiO core-shell heterojunction interface with highly lattice matching, numerous reaction sites and unique interfacial electronic structure as highly active and stable electrocatalysts for OER, HER and ORR to achieve high-performance driven water splitting and rechargeable Zn-air batteries.



## Influence of MnO<sub>x</sub> deposition on TiO<sub>2</sub> nanotube arrays for electrooxidation

Kaihang Zhang\*, Yuanzheng Zhang, Su Liu, Xin Tong, Junfeng Niu, Dong Wang, Junchen Yan, Zhaoyang Xiong, John Crittenden ..... 612

Narrow bandgap manganese oxide(MnO<sub>x</sub>) was composited with TiO<sub>2</sub> nanotube arrays(TiO<sub>2</sub> NTAs) that in-situ oxidized on porous Ti sponge, forming the MnO<sub>x</sub>-TiO<sub>2</sub> NTAs anode. Quantitative characterizations reveal the design and application of high-performance materials for Electrochemical advanced oxidation processes(EAOPs).

