



# Chinese Journal of Catalysis

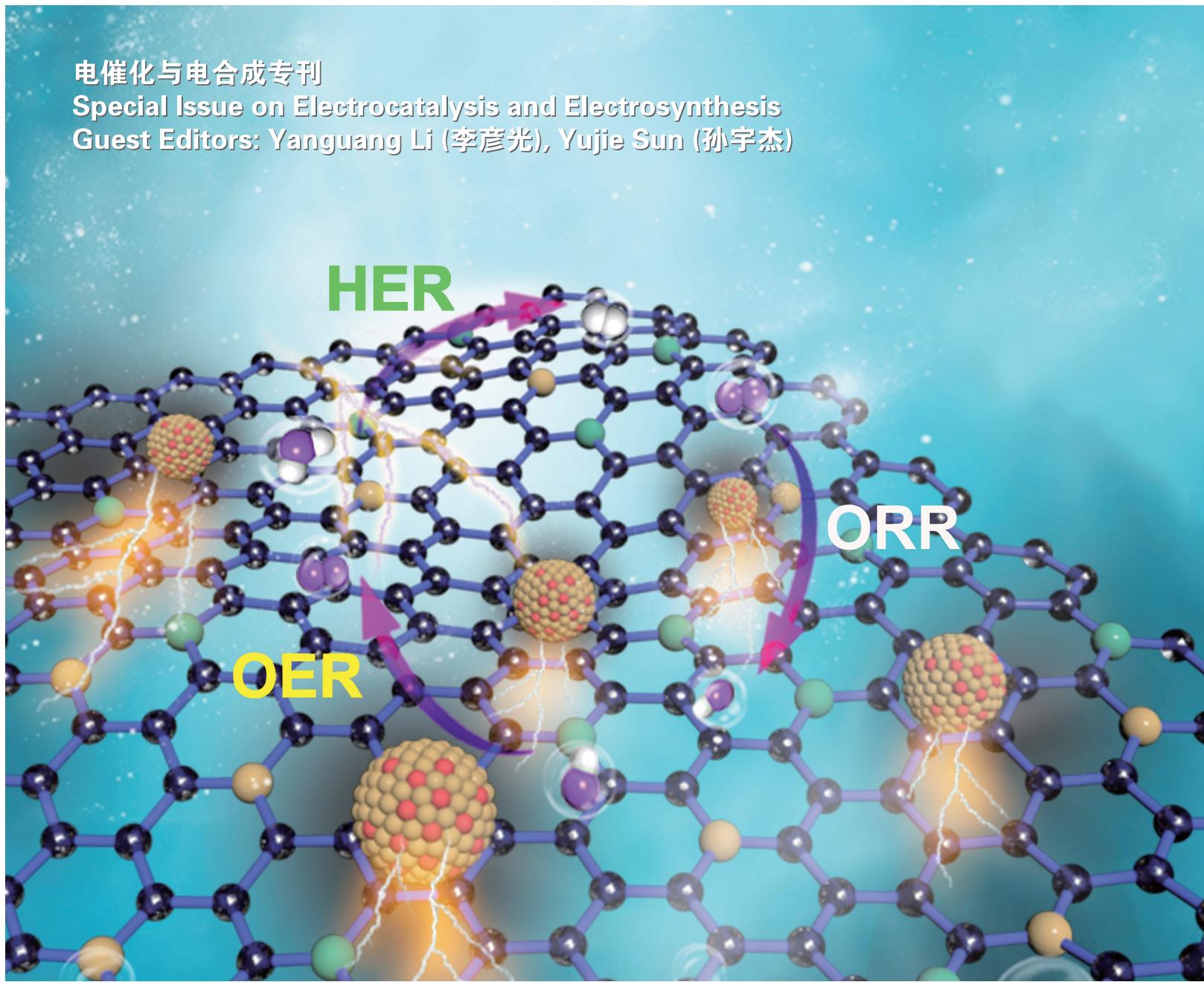
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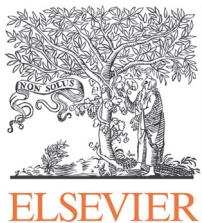
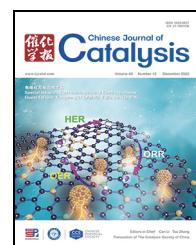
Volume 43 | Number 12 | December 2022

电催化与电合成专刊

Special Issue on Electrocatalysis and Electrosynthesis

Guest Editors: Yanguang Li (李彦光), Yujie Sun (孙宇杰)



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## Special Issue on Electrocatalysis and Electrosynthesis

Guest Editors: Yanguang Li, Yujie Sun

### Chinese Journal of Catalysis

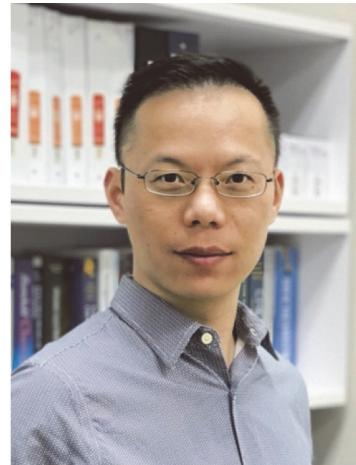
#### Graphical Contents

#### Editorial

*Chin. J. Catal.*, 2022, 43: 2937 doi: 10.1016/S1872-2067(22)64182-2

#### Preface to the special issue on electrocatalysis and electrosynthesis

Yanguang Li, Yujie Sun

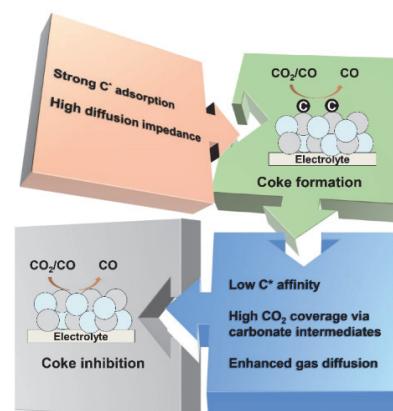
*Soochow University, China; University of Cincinnati, United States*

#### Perspective

*Chin. J. Catal.*, 2022, 43: 2938–2945 doi: 10.1016/S1872-2067(22)64120-2

#### Overcoming coke formation in high-temperature CO<sub>2</sub> electrolysis

Tongbao Wang, Guangtai Han, Ziyun Wang \*, Yuhang Wang \*  
*Soochow University, China; University of Auckland, New Zealand*



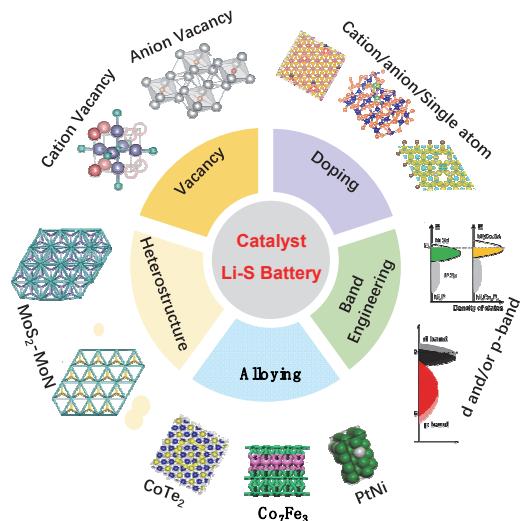
This perspective paper outlines the coking mechanism during high-temperature CO<sub>2</sub> electroreduction in solid oxide electrochemical cells, and discusses the strategies to overcome coke formation and accelerate the implementation of high-temperature CO<sub>2</sub> electroreduction in practice.

## Reviews

*Chin. J. Catal.*, 2022, 43: 2946–2965 doi: 10.1016/S1872-2067(21)63984-0

### Recent progress in electronic modulation of electrocatalysts for high-efficient polysulfide conversion of Li-S batteries

Pan Zeng, Cheng Yuan, Genlin Liu, Jiechang Gao, Yanguang Li \*,  
Liang Zhang \*  
*Soochow University*

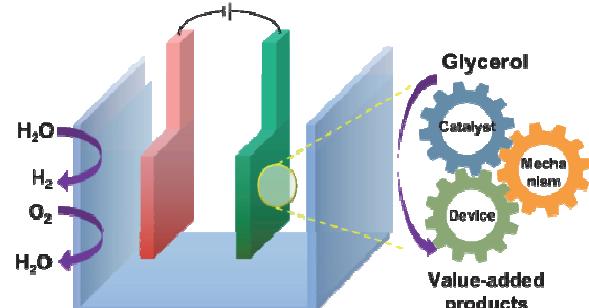


We have summarized the fascinating strategies for regulating the electronic structure of electrocatalysts to accelerate sulfur redox conversion, which could significantly improve the electrochemical performance of Li-S batteries.

*Chin. J. Catal.*, 2022, 43: 2966–2986 doi: 10.1016/S1872-2067(22)64121-4

### Recent advances in glycerol valorization via electrooxidation: Catalyst, mechanism and device

Jianxiang Wu, Xuejing Yang \*, Ming Gong \*  
*Fudan University; East China University of Science and Technology*

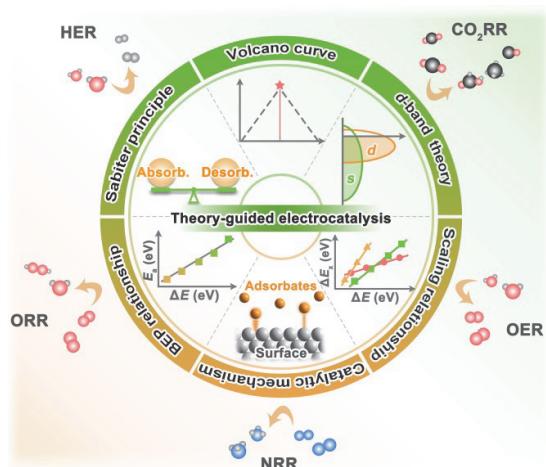


Recent advances of catalyst designs, mechanistic understandings and assembled devices for the electrocatalytic glycerol oxidation into value-added products are reviewed. The detailed activities, selectivities and reaction pathways on different catalysts are summarized.

*Chin. J. Catal.*, 2022, 43: 2987–3018 doi: 10.1016/S1872-2067(22)64103-2

### Theory-guided electrocatalyst engineering: From mechanism analysis to structural design

Mingcheng Zhang, Kexin Zhang, Xuan Ai, Xiao Liang, Qi Zhang,  
Hui Chen \*, Xiaoxin Zou \*  
*Jilin University*

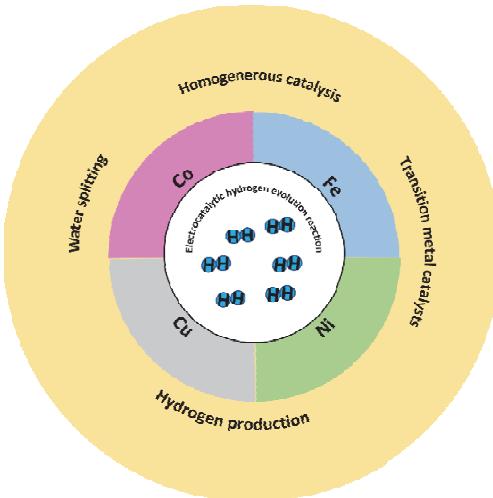


The theory-based efforts used to elucidate catalytic mechanism and address the central challenges facing toward HER, OER, ORR, CO<sub>2</sub>RR and NRR are highlighted. Particular attention is paid to the progress in various types of descriptors for understanding the underlying structure-activity relationships.

*Chin. J. Catal.*, 2022, 43: 3019–3045 doi: 10.1016/S1872-2067(22)64150-0

### Rational development of molecular earth-abundant metal complexes for electrocatalytic hydrogen production

John Daniel McCool, Shiyuan Zhang, Inen Cheng, Xuan Zhao \*  
*The University of Memphis, United States*

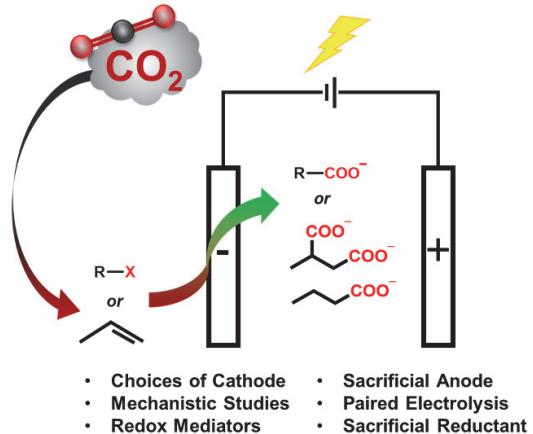


Electrocatalytic hydrogen evolution by molecular metal complexes of Fe, Ni, Co and Cu is briefly discussed to provide insight into catalyst design and structure-function correlations in hydrogen catalysis.

*Chin. J. Catal.*, 2022, 43: 3046–3061 doi: 10.1016/S1872-2067(22)64180-9

### Toward green syntheses of carboxylates: Considerations of mechanisms and reactions at the electrodes for electrocarboxylation of organohalides and alkenes

Teera Chantarojsiri \*, Tassaneewan Soisuwan,  
 Pornwimon Kongkiatkrai  
*Mahidol University, Thailand*

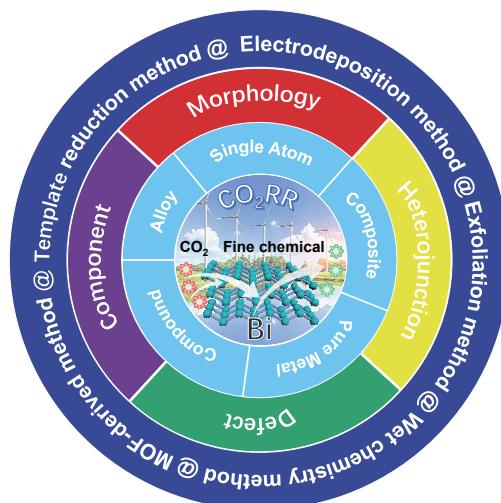


Combining CO<sub>2</sub> to halides or alkenes by electricity to form carboxylates requires a lot of experimental components. This minireview describes electrocarboxylation processes for organohalides and alkenes which include mechanistic studies and choices of electrodes.

*Chin. J. Catal.*, 2022, 43: 3062–3088 doi: 10.1016/S1872-2067(22)64132-9

### Rational design of bismuth-based catalysts for electrochemical CO<sub>2</sub> reduction

Bo Zhang, Yunzhen Wu, Panlong Zhai, Chen Wang, Licheng Sun,  
 Jungang Hou \*  
*Dalian University of Technology, China;*  
*Westlake University, China;*  
*KTH Royal Institute of Technology, Sweden*



The electrochemical CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR) is a promising way to avoid the negative effect brought by the greenhouse effect. This review highlights the development and application of bismuth-based catalysts in the field of CO<sub>2</sub>RR from three points: categories, synthetic approaches and optimization strategies.

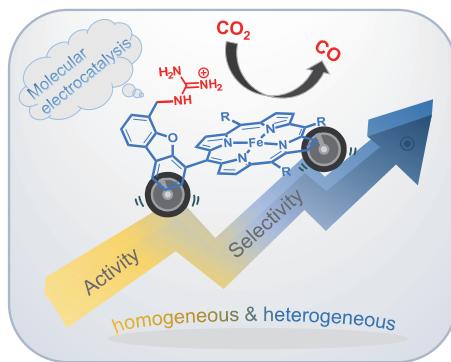
## Communications

*Chin. J. Catal.*, 2022, 43: 3089–3094 doi: 10.1016/S1872-2067(21)63957-8

### Iron porphyrin with appended guanidyl group for significantly improved electrocatalytic carbon dioxide reduction activity and selectivity in aqueous solutions

Hongbo Guo, Zuozhong Liang, Kai Guo, Haitao Lei, Yabo Wang,  
Wei Zhang, Rui Cao \*  
*Shaanxi Normal University*

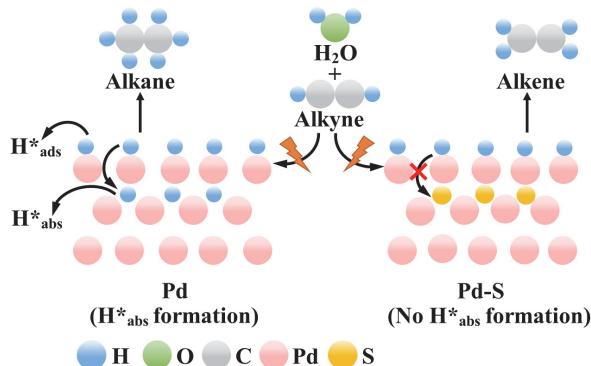
The design and synthesis of iron porphyrin **1** with an appended guanidyl group for significantly improved electrocatalytic carbon dioxide reduction activity and selectivity in both homogeneous and heterogeneous conditions.



*Chin. J. Catal.*, 2022, 43: 3095–3100 doi: 10.1016/S1872-2067(22)64145-7

### Unveiling subsurface hydrogen inhibition for promoting electrochemical transfer semihydrogenation of alkynes with water

Qi Hao, Yongmeng Wu \*, Cuibo Liu, Yanmei Shi, Bin Zhang \*  
*Tianjin University*

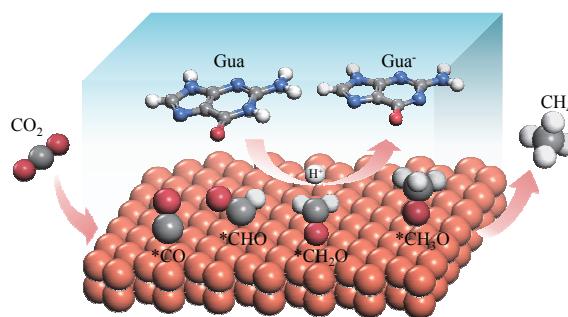


Sulfur-modified Pd nanowires (Pd-S NWs) are synthesized by a solid-solution interface sulfuration method. The introduction of S prevents the diffusion of surface adsorbed hydrogen ( $H^{*}_{ads}$ ) into the Pd lattice to form unselective subsurface ( $H^{*}_{abs}$ ). Potential-independent electrocatalytic alkyne semihydrogenation with 98% alkenes selectivity is realized on the Pd-S catalyst.

*Chin. J. Catal.*, 2022, 43: 3101–3106 doi: 10.1016/S1872-2067(22)64113-5

### Guanine-regulated proton transfer enhances $\text{CO}_2$ -to- $\text{CH}_4$ selectivity over copper electrode

Jun Gong, Jimmeng Li, Chang Liu, Fengyuan Wei, Jinlong Yin, Wenzheng Li, Li Xiao, Gongwei Wang \*, Juntao Lu, Lin Zhuang \*  
*Wuhan University*



Several purines are modified on Cu electrodes to regulate the surface proton delivery in  $\text{CO}_2$  reduction. The  $\text{CH}_4$  production is remarkably enhanced after the modification of guanine, due to its moderate proton transfer capability.

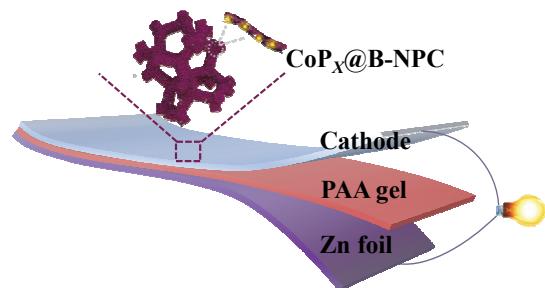
## Articles

*Chin. J. Catal.*, 2022, 43: 3107–3115 doi: 10.1016/S1872-2067(21)64047-0

**In-situ formation of cobalt phosphide nanoparticles confined in three-dimensional porous carbon for high-performing zinc-air battery and water splitting**

Xinxin Shu, Maomao Yang, Miaomiao Liu, Huaisheng Wang,  
Jintao Zhang \*

*Shandong University;  
Liaocheng University*

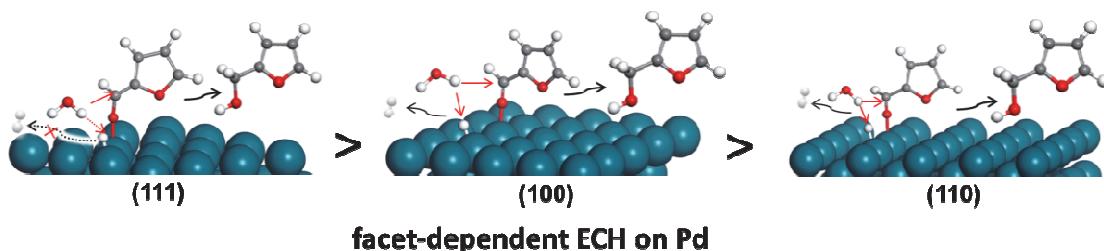


Three-dimensional porous carbon composites embedded with cobalt phosphide nanocrystallites are proposed to enhance the performance of Zn-air batteries and water splitting.

*Chin. J. Catal.*, 2022, 43: 3116–3125 doi: 10.1016/S1872-2067(22)64097-X

**Facet dependence of electrocatalytic furfural hydrogenation on palladium nanocrystals**

Wenbiao Zhang, Yanghao Shi, Yang Yang, Jingwen Tan, Qingsheng Gao \*  
*Jinan University; South China University of Technology*

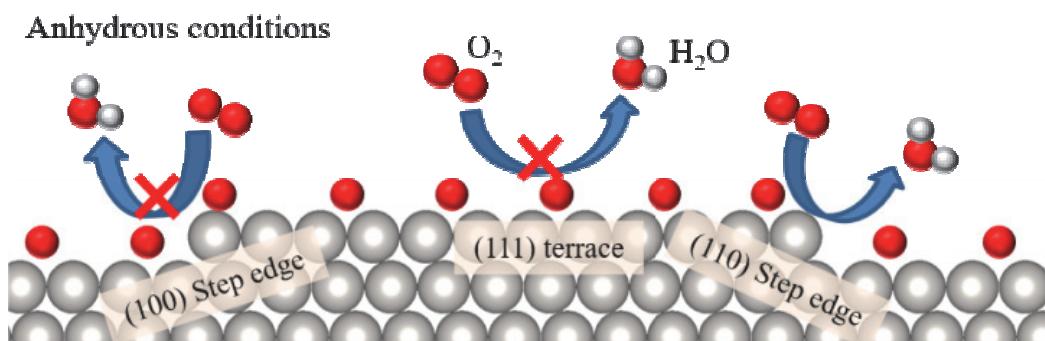


The facet dependence of electrocatalytic furfural hydrogenation is demonstrated on Pd nanocrystals and can be correlated with the difference between the binding energies of chemisorbed hydrogen and furfural based on a competitive adsorption Langmuir-Hinshelwood mechanism.

*Chin. J. Catal.*, 2022, 43: 3126–3133 doi: 10.1016/S1872-2067(22)64125-1

**Density functional theory study of active sites and reaction mechanism of ORR on Pt surfaces under anhydrous conditions**

Guangdong Liu, Huiqiu Deng \*, Jeffrey Greeley, Zhenhua Zeng \*  
*Hunan University, China; Purdue University, United States*



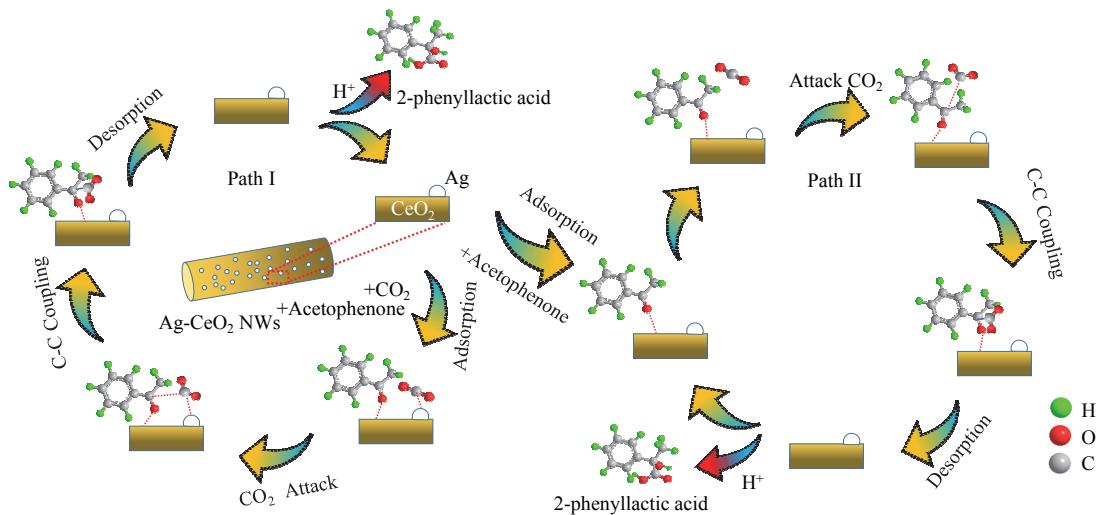
(110) type step edge can stabilize O<sub>2</sub> adsorption and decrease O<sub>2</sub> dissociation barrier because of a unique configuration of accumulated O, which is likely the active site for the oxygen reduction reaction under anhydrous conditions.

*Chin. J. Catal.*, 2022, 43: 3134–3141 doi: 10.1016/S1872-2067(22)64116-0

### Efficient CO<sub>2</sub> fixation with acetophenone on Ag-CeO<sub>2</sub> electrocatalyst by a double activation strategy

Anxiang Guan, Yueli Quan, Yangshen Chen, Zhengzheng Liu, Junbo Zhang, Miao Kan, Quan Zhang, Haoliang Huang, Linping Qian, Linjuan Zhang, Gengfeng Zheng \*

*Fudan University; Shanghai Institute of Applied Physics, Chinese Academy of Sciences*

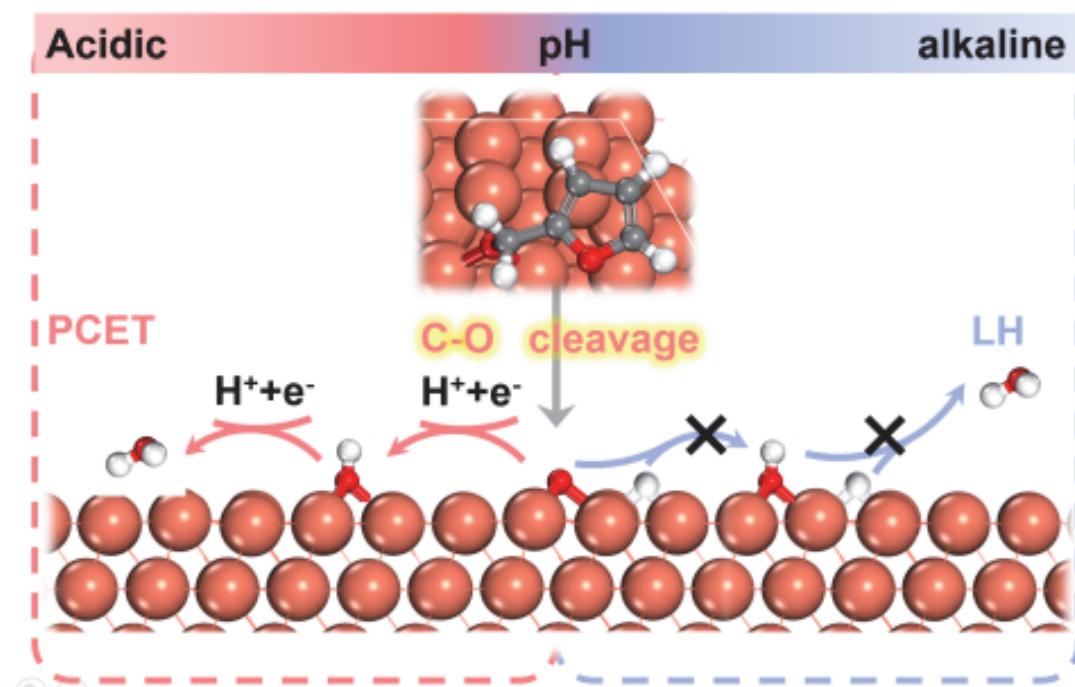


This paper realizes the important role of minimizing the overpotential difference between CO<sub>2</sub> and organic substrate molecules in the CO<sub>2</sub>-involved electrocarboxylation reaction.

*Chin. J. Catal.*, 2022, 43: 3142–3153 doi: 10.1016/S1872-2067(22)64119-6

### pH-Induced selective electrocatalytic hydrogenation of furfural on Cu electrodes

Ling Zhou, Yingying Li, Yuxuan Lu, Shuangyin Wang, Yuqin Zou \*  
*Hunan University; Shenzhen Institute of Hunan University*

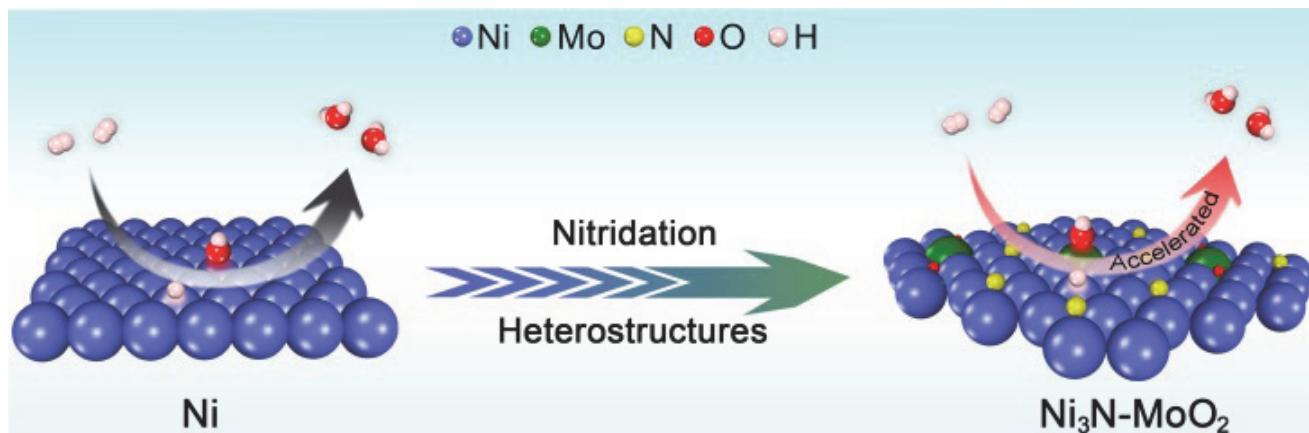


The O atom, produced by direct cleavage of C–O bond, leaves rapidly through proton-coupled electron transfer at Low pH. The large barrier of H<sub>ad</sub> transfer path avoids hydrogenolysis in alkaline.

*Chin. J. Catal.*, 2022, 43: 3154–3160 doi: 10.1016/S1872-2067(22)64126-3

### Enhancing hydrogen electrocatalytic oxidation on $\text{Ni}_3\text{N}/\text{MoO}_2$ in-plane heterostructures in alkaline solution

Lulu An, Shaofeng Deng, Xuyun Guo, Xupo Liu, Tonghui Zhao, Ke Chen, Ye Zhu, Yuxi Fu, Xu Zhao \*, Deli Wang \*  
*Huazhong University of Science and Technology; The Hong Kong Polytechnic University*

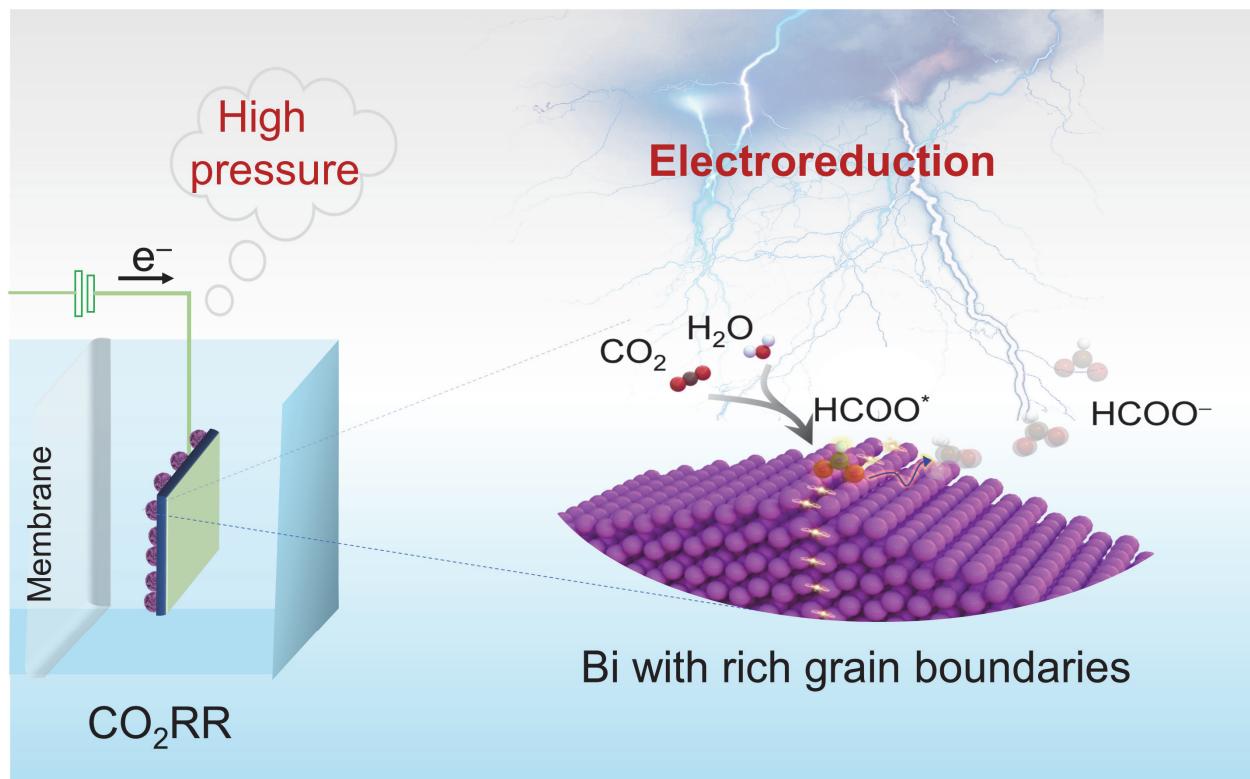


Due to the simultaneous modulated of H and OH adsorption caused by the in-plane heterostructures and nitride structures,  $\text{Ni}_3\text{N}/\text{MoO}_2$  catalysts exhibited an accelerated catalytic process for hydrogen oxidation reaction in alkaline electrolytes.

*Chin. J. Catal.*, 2022, 43: 3161–3169 doi: 10.1016/S1872-2067(22)64131-7

### Bismuth nanosheets with rich grain boundaries for efficient electroreduction of $\text{CO}_2$ to formate under high pressures

Sunhong Ruan, Biao Zhang, Jinhan Zou, Wanfu Zhong, Xiaoyang He, Jinhai Lu, Qinghong Zhang \*, Ye Wang, Shunji Xie \*  
*Xiamen University;*  
*Innovation Laboratory for Sciences and Technologies of Energy Materials of Fujian Province (IKKEM)*

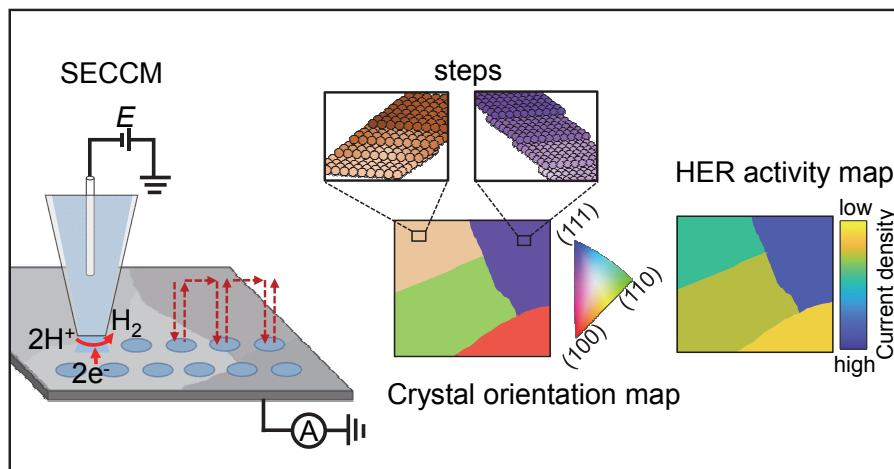


Metallic Bi nanosheets with rich grain boundaries derived from  $\text{BiPO}_4$  nanopolyhedrons in neutral solution under high  $\text{CO}_2$  pressures exhibit a high activity and selectivity for electrocatalytic reduction of  $\text{CO}_2$  to formate in high-pressure H-cell.

*Chin. J. Catal.*, 2022, 43: 3170–3176 doi: 10.1016/S1872-2067(22)64158-5

### Mapping the kinetics of hydrogen evolution reaction on Ag via pseudo-single-crystal scanning electrochemical cell microscopy

Yufei Wang, Mingyang Li, Emma Gordon, Hang Ren \*  
The University of Texas at Austin, United States; Miami University, United States

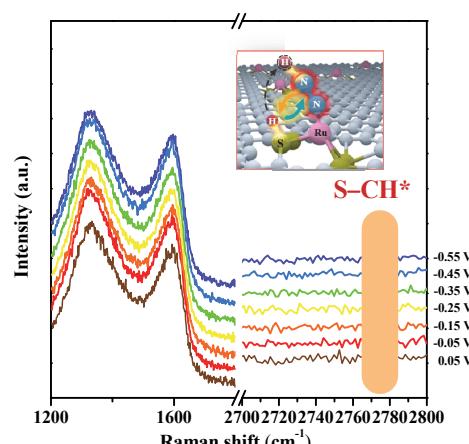


SECCM coupled with colocalized EBSD as a method to directly measure the HER activity on silver to reveal its relationship between activity and crystal orientation.

*Chin. J. Catal.*, 2022, 43: 3177–3186 doi: 10.1016/S1872-2067(22)64136-6

### Dual-site collaboration boosts electrochemical nitrogen reduction on Ru-S-C single-atom catalyst

Liuqing Yang, Chuanqi Cheng, Xun Zhang, Cheng Tang, Kun Du, Yuanyuan Yang, Shan-Cheng Shen, Shi-Long Xu, Peng-Fei Yin \*, Hai-Wei Liang, Tao Ling \*  
Tianjin University, China;  
The University of Adelaide, Australia;  
University of Science and Technology of China, China

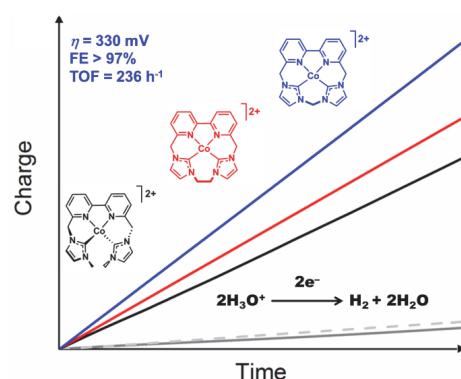


Using *in situ* Raman spectroscopy and dynamic kinetic effect, we experimentally confirmed the positive effect of the Ru/S dual-site mechanism on eNRR over a model Ru-S-C single-atom catalyst.

*Chin. J. Catal.*, 2022, 43: 3187–3194 doi: 10.1016/S1872-2067(22)64151-2

### Electrocatalytic hydrogen evolution from water at low overpotentials with cobalt complexes supported by redox-active bipyridyl-NHC donors

Lizhu Chen, Xiaojun Su, Jonah W. Jurss \*  
University of Mississippi, United States



Three cobalt complexes bearing tunable, redox-active bipyridyl-*N*-heterocyclic carbene-based ligands are studied for electrocatalytic hydrogen evolution from aqueous solutions. High Faradaic efficiencies at low overpotentials are achieved, and a structure-activity relationship is revealed where the smallest macrocycle performs best overall.



## 电催化与电合成专刊

客座主编：李彦光，孙宇杰

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Lizhu Chen, Xiaojun Su, Jonah W. Jurss

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