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# Chinese Journal of Catalysis

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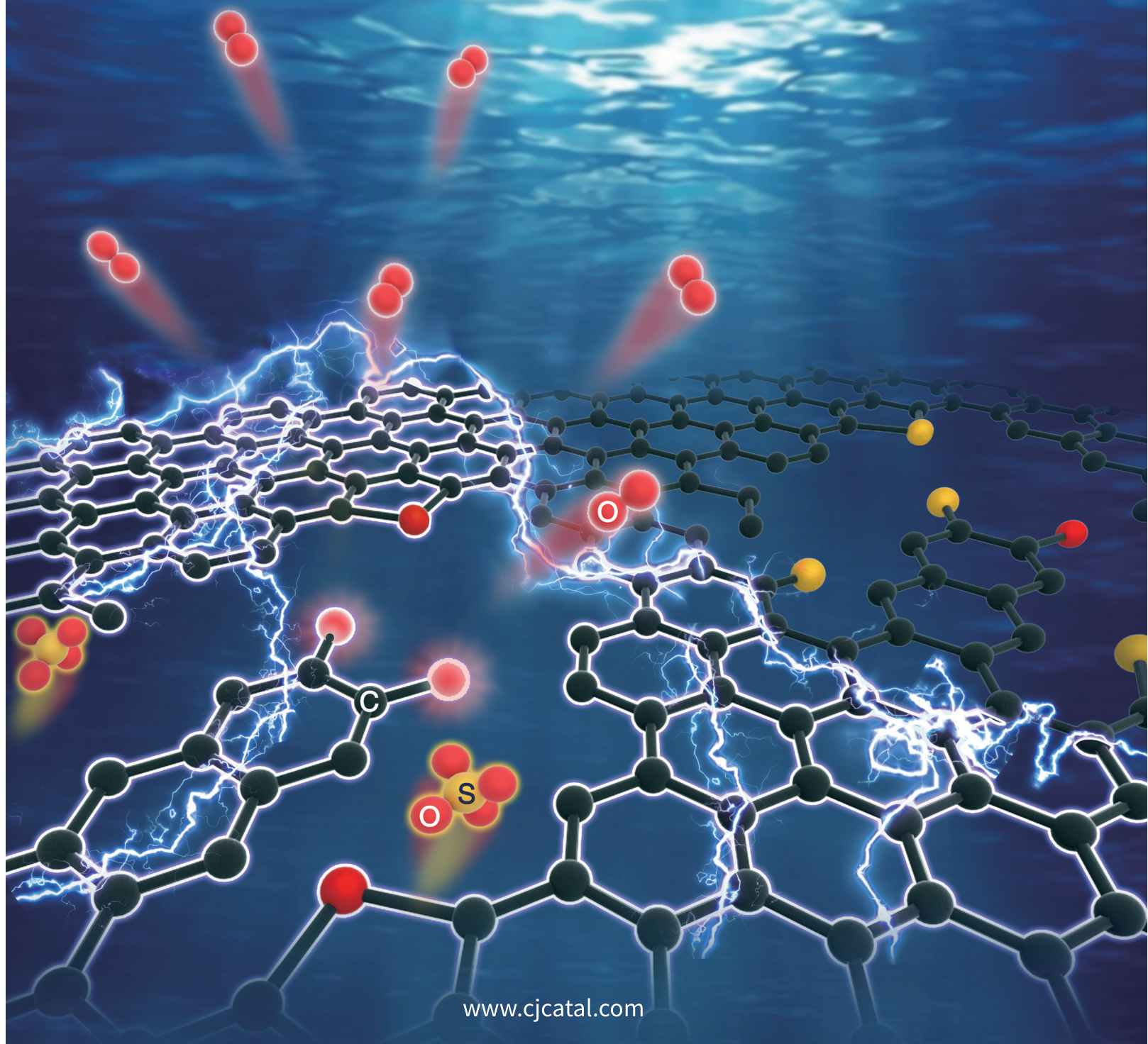
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April 2023

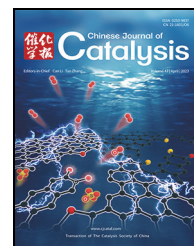
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## Chinese Journal of Catalysis

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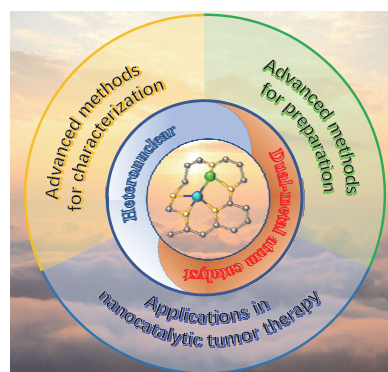
#### Reviews

*Chin. J. Catal.*, 2023, 47: 1–31 doi: 10.1016/S1872-2067(22)64207-4

#### Heteronuclear dual-metal atom catalysts for nanocatalytic tumor therapy

Jingyi Han, Jingqi Guan \*  
Jilin University

In this review, we introduce how to construct and characterize heteronuclear dual-atom catalysts and emphatically discuss their application in the field of nanocatalytic tumor therapy.

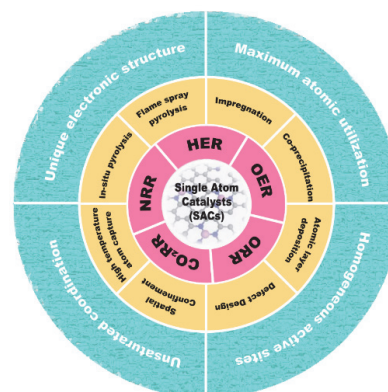


*Chin. J. Catal.*, 2023, 47: 32–66 doi: 10.1016/S1872-2067(23)64392-X

#### Syntheses and applications of single-atom catalysts for electrochemical energy conversion reactions

Qi-Ni Zhan, Ting-Yu Shuai, Hui-Min Xu, Chen-Jin Huang, Zhi-Jie Zhang, Gao-Ren Li \*  
Sichuan University

Single-atom catalysts (SACs), a class of heterogeneous catalysts, have many characteristics, such as a high atom utilization rate and unsaturated coordination. In this paper, we focus on the development of preparation methods for obtaining SACs, including top-down and bottom-up approaches, and the application of some SACs in various electrochemical energy conversion reactions in recent years.

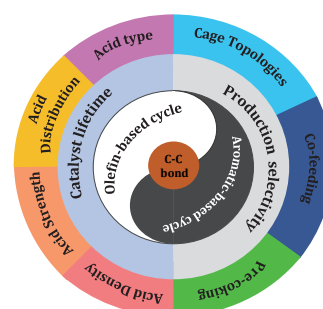


*Chin. J. Catal.*, 2023, 47: 67–92 doi: 10.1016/S1872-2067(22)64209-8

#### Reaction mechanism of methanol-to-hydrocarbons conversion: Fundamental and application

Runze Liu, Xue Shao, Chang Wang, Weili Dai \*, Naijia Guan  
Nankai University

Herein, recent progress in the reaction mechanism of MTH conversion, including the formation and evolution of the first C–C bond species, is emphasized. Based on the reaction mechanism, the catalyst design and optimization for enhancing the product selectivity and catalyst lifetime, are also highlighted.





*Chin. J. Catal.*, 2023, 47: 93–120 doi: 10.1016/S1872-2067(23)64396-7

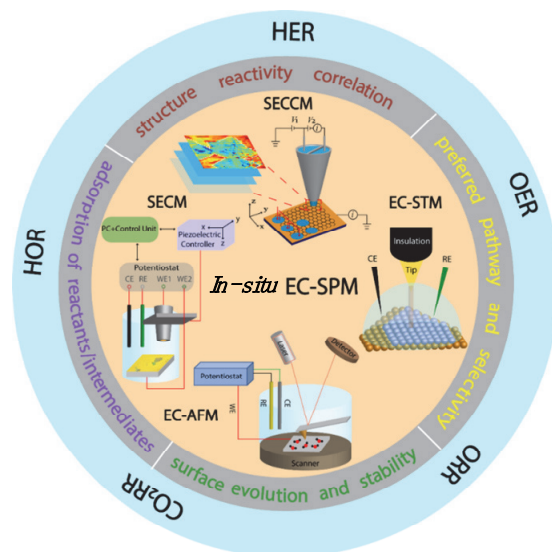
### Advanced *in-situ* electrochemical scanning probe microscopies in electrocatalysis

Dan-Qing Liu, Bingxing Zhang, Guoqiang Zhao, Jian Chen, Hongge Pan, Wenping Sun \*

Zhejiang University;

Xi'an Technological University

In this review, we describe a systematic framework that clarifies the recent progress in *in situ* electrochemical scanning probe microscopy (EC-SPMs) techniques for electrocatalytic applications. This study aims to provide nanoscale insights into the local physiochemical properties and structure-activity correlation that allows the electrocatalysis mechanism and rational design of highly efficient electrocatalysts for energy conversion and storage to be explained.



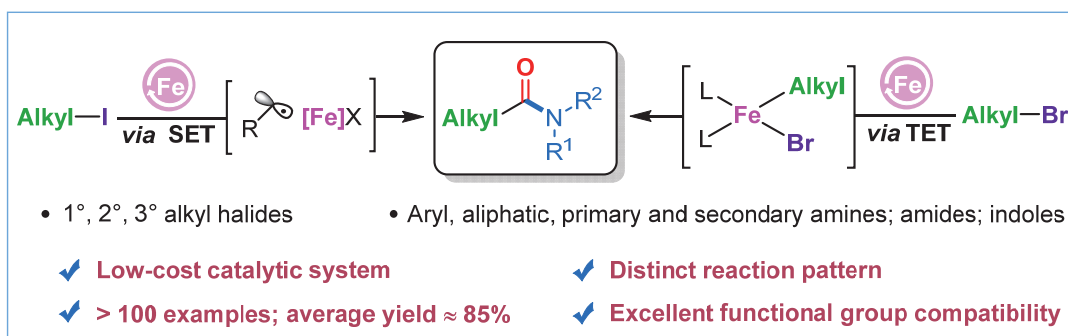
## Communication

*Chin. J. Catal.*, 2023, 47: 121–128 doi: 10.1016/S1872-2067(22)64208-6

### SET or TET? Iron-catalyzed aminocarbonylation of unactivated alkyl halides with amines, amides, and indoles *via* a substrate dependent mechanism

Han-Jun Ai, Fengqian Zhao, Xiao-Feng Wu \*

Leibniz-Institut für Katalyse e.V., Germany; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China



A robust iron-catalyzed carbonylative coupling of alkyl halides with amines, amides, and indoles has been developed. Remarkably, this approach also represents the example on Fe-catalyzed aminocarbonylation of alkyl halides.

## Articles

*Chin. J. Catal.*, 2023, 47: 129–137 doi: 10.1016/S1872-2067(23)64394-3

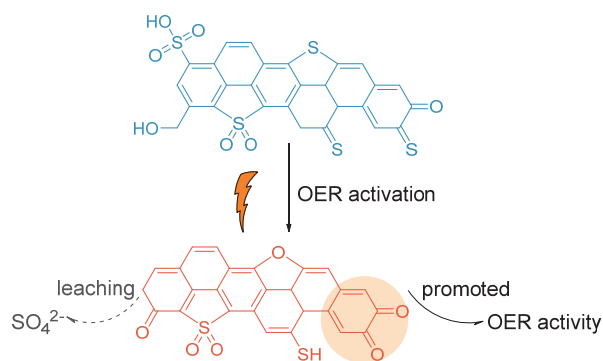
### Unveiling inactive sulfur residue and benzoquinone moiety formation in sulfur-doped carbon for water electrooxidation

Zhipu Zhang, Shanshan Lu, Bin Zhang \*, Yanmei Shi \*

Tianjin University;

Collaborative Innovation Center of Chemical Science and Engineering

Part of the S dopant of S-doped carbon material is dissolved in the form of  $\text{SO}_4^{2-}$  during the OER process, and the newly generated benzoquinone moiety is identified as the real OER active species through multiple characterizations.

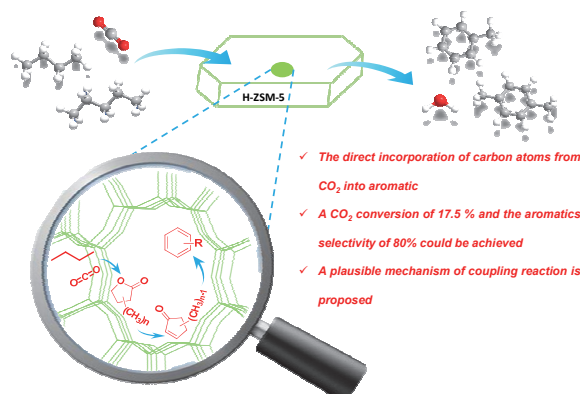


*Chin. J. Catal.*, 2023, 47: 138–149 doi: 10.1016/S1872-2067(23)64416-X

### An efficient way to use CO<sub>2</sub> as chemical feedstock by coupling with alkanes

Changcheng Wei, Wenna Zhang, Kuo Yang, Xiu Bai, Shutao Xu,  
Jinzhe Li \*, Zhongmin Liu \*  
Dalian Institute of Chemical Physics, Chinese Academy of Sciences;  
University of Chinese Academy of Sciences;  
Dalian University of Technology

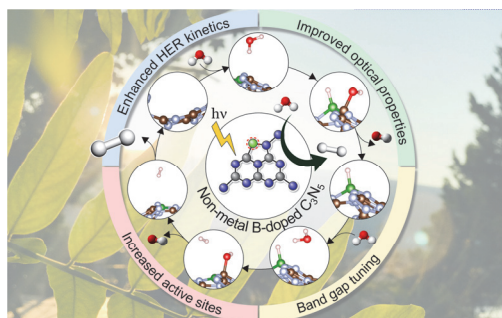
Coupling conversion of CO<sub>2</sub> and light alkanes to aromatics over HZSM-5 is an efficient way to use CO<sub>2</sub> as carbon resources.



*Chin. J. Catal.*, 2023, 47: 150–160 doi: 10.1016/S1872-2067(23)64417-1

### 2D carbon nitrides: Regulating non-metal boron-doped C<sub>3</sub>N<sub>5</sub> for elucidating the mechanism of wide pH range photocatalytic hydrogen evolution reaction

Sue-Faye Ng, Xingzhu Chen, Joel Jie Foo, Mo Xiong \*, Wee-Jun Ong \*  
Xiamen University Malaysia, Malaysia; King Abdullah University of Science and Technology, Saudi Arabia; Xi'an Jiaotong University, China;  
Xiamen University, China; Shenzhen Research Institute of Xiamen University, China; Gulei Innovation Institute, Xiamen University, China

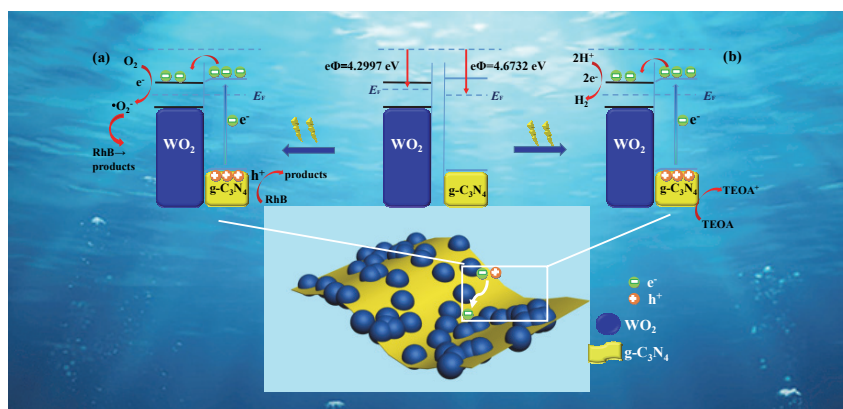


Density functional theory calculation was conducted on boron-doped C<sub>3</sub>N<sub>5</sub> systems to study the dopant effect on the hydrogen evolution reaction (HER) mechanism. The boron-dopant reduced the HER kinetic barrier and improved the system properties.

*Chin. J. Catal.*, 2023, 47: 161–170 doi: 10.1016/S1872-2067(22)64210-4

### Metallic WO<sub>2</sub>-decorated g-C<sub>3</sub>N<sub>4</sub> nanosheets as noble-metal-free photocatalysts for efficient photocatalysis

Ning Li \*, Xueyun Gao, Junhui Su, Yangqin Gao, Lei Ge \*  
China University of Petroleum Beijing



This work designs metallic WO<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> nanocomposite with a highly-efficient photocatalytic performance, resulting from the metal-like behaviour of WO<sub>2</sub> to quickly capture and transfer photogenerated electrons.



*Chin. J. Catal.*, 2023, 47: 171–180 doi: 10.1016/S1872-2067(23)64397-9

### Vinylene-linked covalent organic frameworks with manipulated electronic structures for efficient solar-driven photocatalytic hydrogen production

Zhipeng Xie, Xiubei Yang, Pei Zhang, Xiating Ke, Xin Yuan, Lipeng Zhai \*, Wenbin Wang, Na Qin, Cheng-Xing Cui \*, Lingbo Qu, Xiong Chen \*  
*Fuzhou University;*  
*Zhongyuan University of Technology;*  
*Henan Institute of Science and Technology;*  
*Zhengzhou University*

A donor-acceptor type vinylene-linked TM-DMA-COF exhibits excellent charge separation and transfer kinetics, low charge recombination and energy barrier for H<sub>2</sub> formation, thereby affording the highest photocatalytic hydrogen evolution activity among a series of COF photocatalysts.

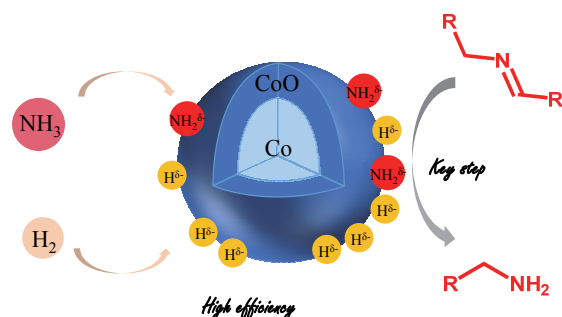


*Chin. J. Catal.*, 2023, 47: 181–190 doi: 10.1016/S1872-2067(22)64196-2

### Co@CoO-catalyzed reductive amination driven by hydride-like NH<sub>2</sub><sup>δ-</sup> species

Wanjun Guo, Zhi-Qiang Wang, Shuang Xiang, Yaxuan Jing \*, Xiaohui Liu, Yong Guo, Xue-Qing Gong \*, Yanqin Wang \*  
*East China University of Science and Technology*

Here, we revealed that the hydride-like NH<sub>2</sub><sup>δ-</sup> from the dissociation of NH<sub>3</sub> over the Co@CoO catalyst can accelerate the ammonolysis of reductive amination intermediate Schiff-base to primary amines.

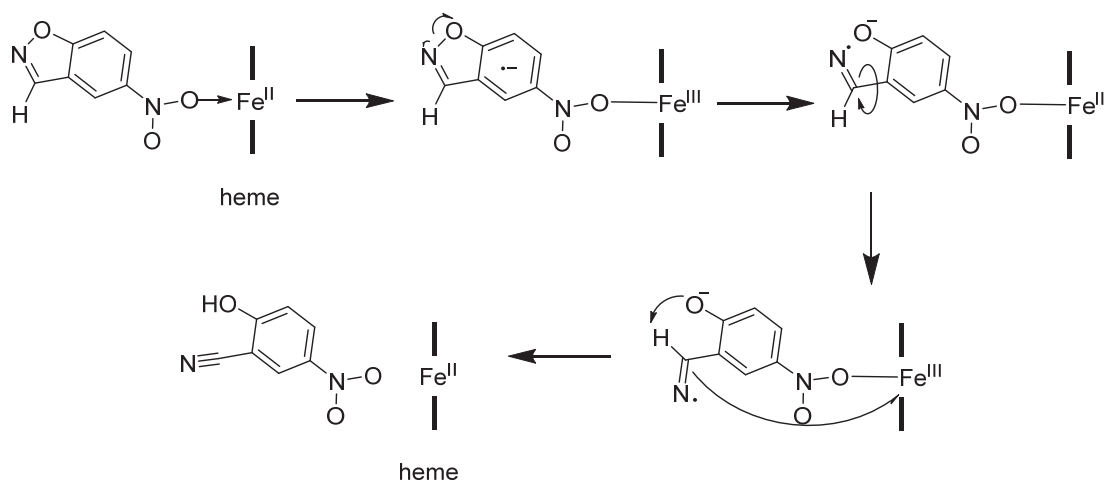


Hydride-like NH<sub>2</sub><sup>δ-</sup> species-driven reductive amination

*Chin. J. Catal.*, 2023, 47: 191–199 doi: 10.1016/S1872-2067(23)64389-X

### Engineering of a P450-based Kemp eliminase with a new mechanism

Aitao Li, Qian Wang, Xitong Song, Xiaodong Zhang, Jian-Wen Huang, Chun-Chi Chen, Rey-Ting Guo \*, Binju Wang \*, Manfred T. Reetz \*  
*Hubei University, China; Xiamen University, China; Max-Planck-Institut für Kohlenforschung, Germany;*  
*Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, China*

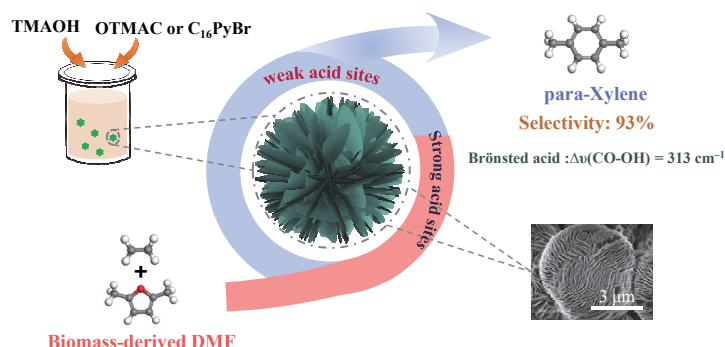


We report a surprising discovery made upon employing new P450-BM3 variants generated by rational enzyme design, which points to the existence of a new and different redox based mechanism. X-ray structural data and theoretical analyses based on MD simulations and QM/MM calculations support this conclusion.

*Chin. J. Catal.*, 2023, 47: 200–213 doi: 10.1016/S1872-2067(22)64200-1

### SCM-36 zeolite nanosheets applied in the production of renewable p-xylene from ethylene and 2,5-dimethylfuran

Duozheng Ma, Xiangcheng Li, Chuang Liu, Caroline Versluis, Yingchun Ye, Zhendong Wang \*, Eelco T. C. Vogt, Bert M. Weckhuysen \*, Weimin Yang \*  
East China University of Science and Technology, China; Sinopec Shanghai Research Institute of Petrochemical Technology, China;  
Utrecht University, the Netherlands

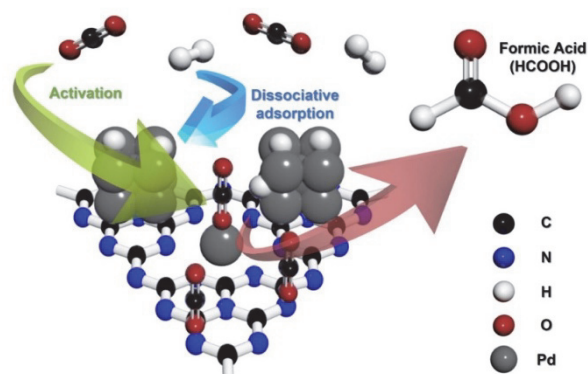


SCM-36, a new aluminosilicate zeolite with a nanosheet morphology, was synthesized with the presences of two organic structure-directing agents. It exhibited up to ~93% selectivity to para-xylene from ethylene and dimethylfuran.

*Chin. J. Catal.*, 2023, 47: 214–221 doi: 10.1016/S1872-2067(22)64202-5

### Synergy between single atoms and nanoclusters of Pd/g-C<sub>3</sub>N<sub>4</sub> catalysts for efficient base-free CO<sub>2</sub> hydrogenation to formic acid

Eun Hyup Kim, Min Hee Lee, Jeehye Kim, Eun Cheol Ra,  
Ju Hyeon Lee, Jae Sung Lee \*  
Ulsan National Institute of Science and Technology (UNIST), Korea

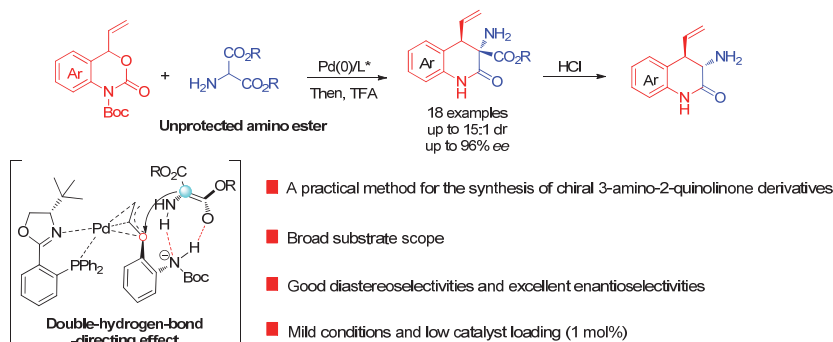


The single atom and nanocluster Pd have different roles in base-free CO<sub>2</sub> hydrogenation to formic acid. Pd/C<sub>3</sub>N<sub>4</sub> catalyst includes two states of Pd that activate reactants CO<sub>2</sub> and H<sub>2</sub> for highest activity in similar reaction condition.

*Chin. J. Catal.*, 2023, 47: 222–228 doi: 10.1016/S1872-2067(23)64390-6

### Enantioselective synthesis of unprotected 2-quinolinone-based cyclic amino acids via sequential palladium-catalyzed asymmetric allylation/desymmetrization

Qian Li, Yan Liu \*, Can Li \*  
Dalian University of Technology; Dalian Institute of Chemical Physics, Chinese Academy of Sciences



Pd(0)-catalyzed enantioselective sequential allylation/desymmetrization is reported for the synthesis of unprotected 2-quinolinone-based cyclic amino acids.

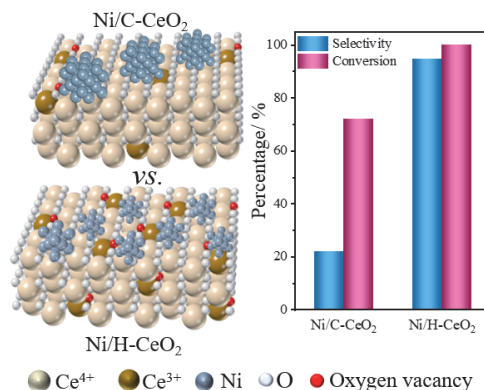


*Chin. J. Catal.*, 2023, 47: 229–242 doi: 10.1016/S1872-2067(23)64401-8

### Ni nanoparticle coupled surface oxygen vacancies for efficient synergistic conversion of palmitic acid into alkanes

Yan Zeng, Hui Wang, Huiru Yang, Chao Juan, Dan Li \*, Xiaodong Wen, Fan Zhang, Ji-Jun Zou, Chong Peng, Changwei Hu  
Sichuan University, Institute of Coal Chemistry;  
Tianjin University;  
Dalian University of Technology

Ni/H-CeO<sub>2</sub> exhibits more excellent catalytic activity than Ni/C-CeO<sub>2</sub> due to the synergistic effect between the small Ni nanoparticles and the rich oxygen vacancy (O<sub>v</sub>), and Ni nanoparticle size was successfully regulated by the O<sub>v</sub> concentration of CeO<sub>2</sub> carriers.

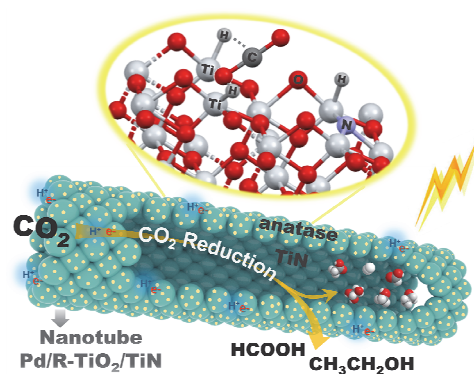


*Chin. J. Catal.*, 2023, 47: 243–253 doi: 10.1016/S1872-2067(23)64395-5

### Photoelectrocatalytic reduction of CO<sub>2</sub> catalyzed by TiO<sub>2</sub>/TiN nanotube heterojunction: Nitrogen assisted active hydrogen mechanism

Yan Wei, Ruizhi Duan, Qiaolan Zhang, Youzhi Cao, Jinyuan Wang, Bing Wang, Wenrui Wan, Chunyan Liu, Jiazang Chen, Hong Gao \*, Huanwang Jing \*  
Lanzhou University;  
Dalian Institute of Chemical Physics, Chinese Academy of Sciences;  
Institute of Coal Chemistry, Chinese Academy of Sciences

The nanotube TiO<sub>2</sub>/TiN heterojunctions with abundant Ti<sup>3+</sup> and oxygen vacancies exhibit high efficiency and selectivity for C<sub>2</sub> products in photoelectrocatalytic CO<sub>2</sub> reduction. The nitrogen-assisted active hydrogen mechanism is verified by operando FTIR and DFT calculations.

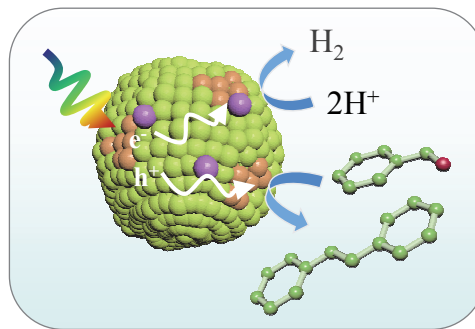


*Chin. J. Catal.*, 2023, 47: 254–264 doi: 10.1016/S1872-2067(23)64393-1

### Co nanoparticles modified phase junction CdS for photoredox synthesis of hydrobenzoin and hydrogen evolution

Meiyu Zhang, Kongming Li, Chunlian Hu, Kangwei Ma, Wanjun Sun, Xianqiang Huang \*, Yong Ding \*  
Lanzhou University;  
Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences;  
Liaocheng University

The cobalt deposited phase junction CdS with co-exposed facets of (001) and (101) (HC-CdS<sub>2</sub>/Co) presents an excellent H<sub>2</sub> evolution activity while the conversion of benzyl alcohol reaches 92% with 97% selectivity of hydrobenzoin.

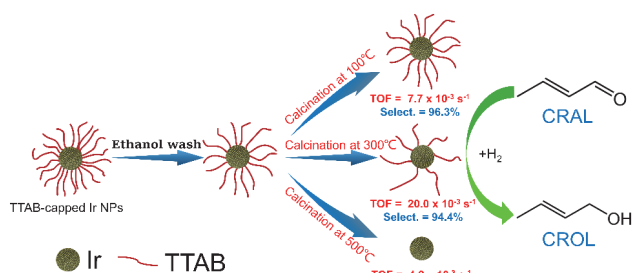


*Chin. J. Catal.*, 2023, 47: 265–277 doi: 10.1016/S1872-2067(23)64399-2

### Hydrogenation of crotonaldehyde over ligand-capped Ir catalysts: Metal-organic interface boosts both activity and selectivity

Yan-Wen Ye, Yi-Ming Hu, Wan-Bin Zheng, Ai-Ping Jia, Yu Wang \*, Ji-Qing Lu \*  
Zhejiang Normal University

The TTAB-capped Ir catalysts are very active and selective for the hydrogenation of crotonaldehyde, due to the enhanced adsorption of crotonaldehyde on the catalyst surface via strong crotonaldehyde-TTAB interaction.



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