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Chinese Journal of Catalysis

Graphical Contents

Account

Chin. J. Catal., 2023, 48: 1–14 doi: 10.1016/S1872-2067(23)64423-7

Strategies for local electronic structure engineering of two-dimensional electrocatalysts

Cheng-Feng Du, Erhai Hu, Hong Yu *, Qingyu Yan * Northwestern Polytechnical University, China; Nanyang Technological University, Singapore

In this account, the strategies adopted for regulating the local electronic structures of 2D electrocatalysts, including heteroatom doping, single-atom loading, and heterojunction, vacancy, and strain engineering are briefly summarized. The relationship between these strategies and electrocatalytic performance is also discussed.



Reviews

Chin. J. Catal., 2023, 48: 15-31 doi: 10.1016/S1872-2067(23)64427-4

Carbon-based catalysts of the oxygen reduction reaction: Mechanistic understanding and porous structures

Wenjing Zhang, Jing Li *, Zidong Wei * Chongqing University



This review systematically summarizes the strategies to regulate the intrinsic activity of the catalytic sites as well as the routes to construct micro-, meso- and macro-porous structures, for enhancing the performances of carbon-based catalysts in oxygen reduction reaction.

Chin. J. Catal., 2023, 48: 32-65 doi: 10.1016/S1872-2067(23)64429-8

Huanhuan Yang, Shiying Li, Qun Xu * Zhengzhou University; Institute of Coal Chemistry, Chinese Academy of Sciences



There are four important steps of inhibition of HER, CO_2 adsorption and activation, CO generation and adsorption, and C–C coupling, need to be considered for promoting CO_2RR -to- C_{2+} . Based on this, surface modifaction of Cu-based electrodes includes hydrophobization, incorporating CO_2 capture materials, halide ions doping, enhancing electric-thermal field, and designing bifunctional catalysts, confinement structures, oxidation states, defects, monatomic Cu, and heterojunction structures.

Chin. J. Catal., 2023, 48: 66-89 doi: 10.1016/S1872-2067(23)64428-6

High-temperature shock synthesis of high-entropy-alloy nanoparticles for catalysis

Yanchang Liu, Xinlong Tian, Ye-Chuang Han *, Yanan Chen *, Wenbin Hu *Tianjin University; Hainan University; Xiamen University*



The characteristics of high-temperature shock (HTS) are matched with those of the fabrication of catalytic high-entropy alloys (HEAs). We present the physicochemical principles of HTS, introduce three typical methods (Joule heating, laser heating, and microwave heating), and review the progress of HEAs prepared by HTS.

Articles

Chin. J. Catal., 2023, 48: 90-100 doi: 10.1016/10.1016/S1872-2067(23)64408-0

Mechanistic and microkinetic study of nonoxidative coupling of methane on Pt-Cu alloy catalysts: From single-atom sites to single-cluster sites

Zheng-Qing Huang, Shu-Yue He, Tao Ban, Xin Gao, Yun-Hua Xu, Chun-Ran Chang * *Xi'an Jiaotong University; Yulin University*



The complex reaction mechanism of nonoxidative coupling of methane (NOCM) on Pt SASs and SCSs is explored and the Pt SASs on Cu(111) are predicted to be more advantageous over the Pt SCSs for NOCM.

Chin. J. Catal., 2023, 48: 101-116 doi: 10.1016/S1872-2067(23)64407-9

Elucidating coke formation and evolution in the catalytic steam reforming of biomass pyrolysis volatiles at different fixed bed locations

Enara Fernandez, Laura Santamaria, Irati García, Maider Amutio, Maite Artetxe, Gartzen Lopez *, Javier Bilbao, Martin Olazar University of the Basque Country, Spain; Basque Foundation for Science, Spain



The mechanisms of coke formation strongly depend on the location in a fixed bed reactor and the reaction time. The nature, morphology and composition of coke deposits affect catalyst stability in the biomass pyrolysis-reforming process.

Chin. J. Catal., 2023, 48: 117–126 doi: 10.1016/S1872-2067(23)64412-2

$Precise\ design\ of\ nickel\ phthalocyanine\ molecular\ structure:\ Optimizing\ electronic\ and\ spatial\ effects\ for\ remarkable\ electrocatalytic\ CO_2\ reduction$

Jingjing Li, Fengwei Zhang *, Xinyu Zhan, Hefang Guo, Han Zhang, Wen-Yan Zan *, Zhenyu Sun *, Xian-Ming Zhang * Shanxi University; Beijing University of Chemical Technology; Taiyuan University of Technology



A set of well-structured molecularly dispersed NiPc-based electrocatalysts was prepared. Among them, the α -NO₂-substituted NiPc exhibited highest FE_{CO} with 99% and wide potential window with FE_{CO} exceeding 91.1% for CO₂RR.

Chin. J. Catal., 2023, 48: 127-136 doi: 10.1016/S1872-2067(23)64411-0

Microenvironment regulation of Ru(bda)L₂ catalyst incorporated in metal-organic framework for effective photo-driven water oxidation

Jianxin Feng, Xuan Li, Yucheng Luo, Zhifang Su, Maoling Zhong, Baolan Yu, Jianying Shi* Sun Yat-Sen University



microenvironment

water-networks around catalysts

proton transport and/or electron transfer in WNA mechanism

The enzyme-like microenvironment, derived from the dissociation of Ru(bda)L2@UiO-66 during photo-driven water oxidation, allows for the cooperative interplay between Ru(bda)L₂, water molecule and phosphate proton mediator required for high efficiency proton and proton-couple electron transfer.

Chin. J. Catal., 2023, 48: 137-149 doi: 10.1016/S1872-2067(23)64422-5

Benzimidazole-based covalent organic framework embedding single-atom Pt sites for visible-light-driven photocatalytic hydrogen evolution

Fangpei Ma, Qingping Tang, Shibo Xi, Guoqing Li, Tao Chen, Xingchen Ling, Yinong Lyu, Yunpeng Liu, Xiaolong Zhao, Yu Zhou *, Jun Wang * Nanjing Tech University, China; Institute of Chemical and Engineering Sciences, Singapore; Institute of High Energy Physics, Chinese Academy of Sciences, China

A benzimidazole-based COF allowed the formation of single-atom Pt sites during an in-situ photo-deposition process, affording a high H2 evolution rate of 115 mmol g⁻¹ h⁻¹ and turnover frequency of 4475.1 h⁻¹ under visible-light irradiation.

Chin. J. Catal., 2023, 48: 150-163 doi: 10.1016/S1872-2067(23)64410-9

Tuning cobalt carbide wettability environment for Fischer-Tropsch to olefins with high carbon efficiency

Peigong Liu, Tiejun Lin *, Lei Guo, Xiaozhe Liu, Kun Gong, Taizhen Yao, Yunlei An, Liangshu Zhong* ShanghaiTech University; Shanghai Advanced Research Institute, Chinese Academy of Sciences;

University of Chinese Academy of Sciences

The local wettability environment is tuned through the physical mixing of cobalt carbide with hydrophobic SiO2, and the suppressed water-gas-shift reaction largely decreases CO₂ selectivity while enhancing activity and olefin selectivity during syngas conversion.





Chin. J. Catal., 2023, 48: 164–174 doi: 10.1016/S1872-2067(23)64402-X

Sn_1Pt single-atom alloy evolved stable $PtSn/nano\mathchar`Al_2O_3$ catalyst for propane dehydrogenation

Yanan Xing, Leilei Kang, Jingyuan Ma, Qike Jiang, Yang Su, Shengxin Zhang, Xiaoyan Xu, Lin Li, Aiqin Wang, Zhi-Pan Liu, Sicong Ma *, Xiao Yan Liu *, Tao Zhang

Dalian Institute of Chemical Physics, Chinese Academy of Sciences; University of Chinese Academy of Sciences;

Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences; Shanghai Advanced Research Institute, Chinese Academy of Sciences; Fudan University

The holistic structural evolution of PtSn/Al₂O₃ during propane dehydrogenation is pictured by using various *in situ* characterizations, in which a highly active Sn₁Pt single-atom alloy accountable for the formation of stable active center of Pt₃Sn intermetallic compound is identified in both experimental and theoretical results.

Chin. J. Catal., 2023, 48: 175–184 doi: 10.1016/S1872-2067(23)64418-3

Facile synthesis of CoSi alloy catalysts with rich vacancies for base- and solvent-free aerobic oxidation of aromatic alcohols

Zhiyue Zhao, Zhiwei Jiang, Yizhe Huang, Mebrouka Boubeche, Valentina G. Matveeva, Hector F. Garces, Huixia Luo, Kai Yan * Sun Yat-Sen University, China; Tver State Technical University, Russian; Brown University, USA



Chin. J. Catal., 2023, 48: 185–194 doi: 10.1016/S1872-2067(23)64415-8

Fe nanoparticles embedded in N-doped porous carbon for enhanced electrocatalytic CO2 reduction and Zn-CO2 battery

Wenqian Yang, Ziqian Xue, Jun Yang, Jiahui Xian, Qinglin Liu, Yanan Fan, Kai Zheng, Peiqin Liao, Hui Su, Qinghua Liu, Guangqin Li*, Cheng-Yong Su*

Sun Yat-Sen University, China; Kyoto University, Japan; University of Science and Technology of China, China



Fe nanoparticles were embedded in *N*-doped porous carbons derived from a pre-modified metal-organic framework, resulting in an Fe@NPC composite with an excellent FE_{CO} of 96.4% at -0.5 V_{RHE} . This catalyst can be employed in a Zn-CO₂ battery, providing a peak power density of 3 mW cm⁻² with good durability.





Chin. J. Catal., 2023, 48: 195-204 doi: 10.1016/S1872-2067(23)64424-9

Enhancing the chemoselective hydrogenation of nitroarenes: Designing a novel surface-strained carbon-based Pt nanocatalyst

Fengwei Zhang *, Hefang Guo, Mengmeng Liu, Yang Zhao, Feng Hong, Jingjing Li, Zhengping Dong *, Botao Qiao * Shanxi University; Dalian Institute of Chemical Physics, Chinese Academy of Sciences; Lanzhou University



The compressive-strained Pt/CNTs-800H catalyst with strong metal-support interaction was prepared *via* a facile and scalable thermal reduction strategy. It displays superior selectivity and stability and is well-suited for the selective hydrogenation of vulnerable nitroarenes.

Chin. J. Catal., 2023, 48: 205-213 doi: 10.1016/S1872-2067(23)64413-4

Computational insights on potential dependence of electrocatalytic synthesis of ammonia from nitrate

Huijuan Jing, Jun Long, Huan Li, Xiaoyan Fu, Jianping Xiao * Dalian Institute of Chemical Physics, Chinese Academy of Sciences; University of Chinese Academy of Sciences



The charge transfer coefficient plays a key role in the potential-dependent product selectivity, so potential-dependent barriers are necessary to more accurately describe the reaction mechanism, activity, and selectivity.

Chin. J. Catal., 2023, 48: 214-223 doi: 10.1016/S1872-2067(23)64398-0

$Phosphine-catalyzed \ photo-induced \ alkoxy carbonylation \ of \ alkyl \ iodides \ with \ phenols \ and \ 1,4-dioxane \ through \ charge-transfer \ complex$

Xing-Wei Gu, Youcan Zhang, Fengqian Zhao, Han-Jun Ai, Xiao-Feng Wu * Leibniz-Institut für Katalyse, Germany; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China



We have developed an interesting phosphine-catalyzed carbonylation by charge-transfer complex through photoactivation under atmospheric pressure of CO. Five-component perfluoroalkylative carbonylation for the synthesis of β -perfluoroalkyl acyloxy esters from unactivated olefins and perfluoroalkyl iodides can be realized as well. Notably, a series of carbon-13 labeled products were also obtained in good to excellent yields by using 1 bar of ¹³CO.

Chin. J. Catal., 2023, 48: 224-234 doi: 10.1016/S1872-2067(23)64419-5

Defect engineering of Fe-N-C single-atom catalysts for oxygen reduction reaction

Run Jiang, Zelong Qiao, Haoxiang Xu *, Dapeng Cao * Beijing University of Chemical Technology



This work reveals the origin of oxygen reduction reaction (ORR) activity of defective Fe-N-C. The intrinsic structure descriptor φ is established to quantitatively predict the ORR activity without requirement of density functional calculations, which provides intuitive guidance to design ORR catalysts by defect engineering.

Chin. J. Catal., 2023, 48: 235–246 doi: 10.1016/S1872-2067(23)64409-2

Activation of partial metal sites in high-entropy oxides for enhancing thermal and electrochemical catalysis

Jinxing Mi, Xiaoping Chen, Yajun Ding, Liangzhu Zhang, Jun Ma, Hui Kang, Xianhong Wu, Yuefeng Liu, Jianjun Chen *, Zhong-Shuai Wu * Dalian Institute of Chemical Physics, Chinese Academy of Sciences; Tsinghua University



The lamellar CuCoNiZnAl-T-NaOH high entropy oxide with activated Cu, Co, and Ni oxides species accompanied with enriched lattice oxygen species displays remarkably improved performance of redox catalysis and Li-O₂ battery.

Chin. J. Catal., 2023, 48: 247-257 doi: 10.1016/S1872-2067(23)64426-2

In-situ adaptive evolution of rhodium oxide clusters into single atoms via mobile rhodium-adsorbate intermediates

Zhengtian Pu, Haibin Yin, Xinlong Ma, Jin Zhao, Jie Zeng * University of Science and Technology of China, China; University of Pittsburgh, USA



During hydroformylation of propene, initially inactive RhO_x clusters on reduced Al_2O_3 evolved into the catalytically active oxygen vacancies and Rh single atoms *via* mobile Rh–CO intermediates.

Chin. J. Catal., 2023, 48: 258-266 doi: 10.1016/S1872-2067(23)64400-6

Magnetic core-shell composites accessed by coordination assembly boost catalytic ${\rm CO}_2$ valorization

Jinpeng Li, Jie Chen, Qingshu Zheng, Bo Tu*, Tao Tu* Fudan University; Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences; Zhengzhou University



Magnetic core-shell nanocomposites were prepared by encapsulating Fe_3O_4 NPs with *N*-heterocyclic carbene metal coordination assemblies, which showed enhanced catalytic activity towards a number of CO_2 transformations. A record turnover number of 1.69×10^6 was achieved in the hydrogenation of CO_2 to formic acid, and the catalyst could be reused for multiple times in the dehydrogenation of ammonium formate.

Chin. J. Catal., 2023, 48: 267–278 doi: 10.1016/S1872-2067(23)64420-1

LSPR-enhanced carbon-coated In₂O₃/W₁₈O₄₉ S-scheme heterojunction for efficient CO₂ photoreduction

Houwei He, Zhongliao Wang, Kai Dai*, Suwen Li*, Jinfeng Zhang* Huaibei Normal University



A carbon-coated $In_2O_3/W_{18}O_{49}$ S-scheme heterojunction photocatalyst with enhanced LSPR effect was successfully constructed. The excellent catalytic performance of the C- $In_2O_3/W_{18}O_{49}$ composite is attributed to the uniform distribution and favorable transfer of carriers at the heterogeneous interface, which is achieved by the carbon coating in the LSPR-enhanced S-scheme heterojunction.

Chin. J. Catal., 2023, 48: 279-289 doi: 10.1016/S1872-2067(23)64414-6

Nanoscale lamination effect by nitrogen-deficient polymeric carbon nitride growth on polyhedral SrTiO₃ for photocatalytic overall water splitting: Synergy mechanism of internal electrical field modulation

Zhidong Wei, Jiawei Yan, Weiqi Guo, Wenfeng Shangguan * Shanghai Jiao Tong Univeristy



 $PCN-SrTiO_3$ composites with laminated structures were formed. The generation of the N-Sr bond could regulate the built-in electrical field of PCN. As a result, the photocatalytic overall water splitting was achieved.







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