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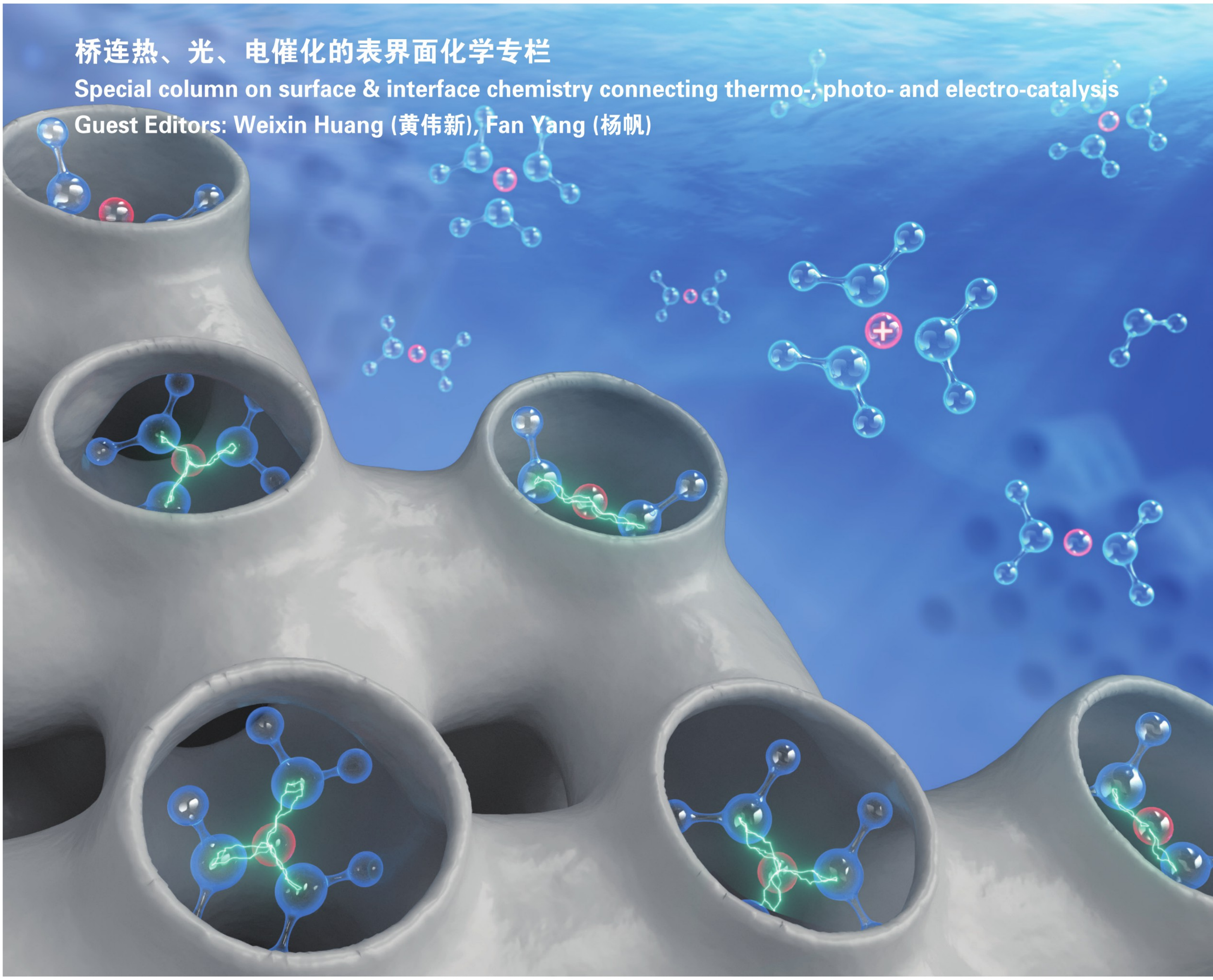

桥连热、光、电催化的表界面化学专栏

Special column on surface & interface chemistry connecting thermo-, photo- and electro-catalysis

Guest Editors: Weixin Huang (黄伟新), Fan Yang (杨帆)

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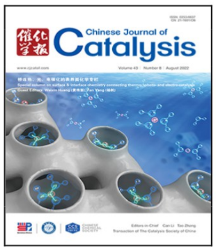


Chinese Journal of Catalysis

Graphical Contents

Special column on surface & interface chemistry connecting thermo-, photo- and electro-catalysis

Chin. J. Catal., 2022, 43: 1963 doi: 10.1016/S1872-2067(22)64135-4 **[Editorial]**

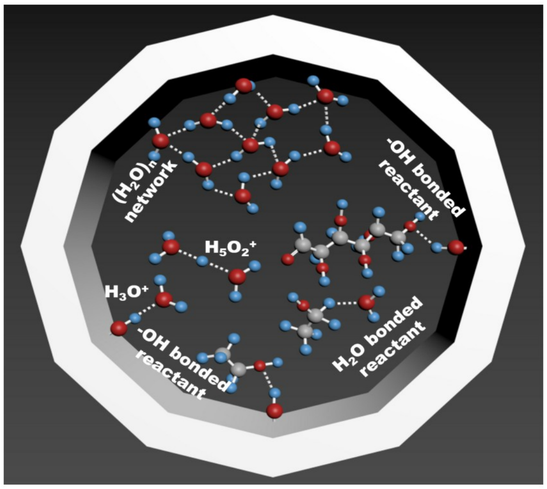
Preface to special column on surface & interface chemistry connecting thermo-, photo- and electro-catalysis

Weixin Huang, Fan Yang (Guest Editors)
University of Science and Technology of China; ShanghaiTech University

Chin. J. Catal., 2022, 43: 1964–1990 doi: 10.1016/S1872-2067(21)64032-9 **[Review]**

A critical assessment of the roles of water molecules and solvated ions in acid-base-catalyzed reactions at solid-water interfaces

Xugang Yang, Zonghui Liu, Guoliang Wei, Yu Gu *, Hui Shi *
Yangzhou University; Changzhou University

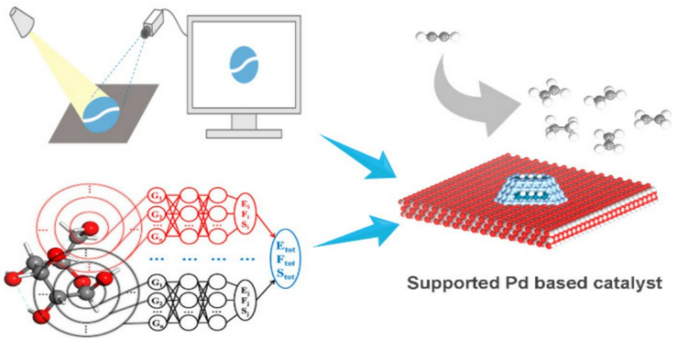


Through illustrative examples, this review highlights the utmost importance of hydrogen-bonding interactions and interfacial ionic species as the main factors underlying acid-base catalysis and the associated solvation effects at the solid-aqueous interfaces.

Chin. J. Catal., 2022, 43: 1991–2000 doi: 10.1016/S1872-2067(21)64036-6 **[Review]**

Selectivity control in alkyne semihydrogenation: Recent experimental and theoretical progress

Xiao-Tian Li, Lin Chen, Cheng Shang, Zhi-Pan Liu *
Fudan University

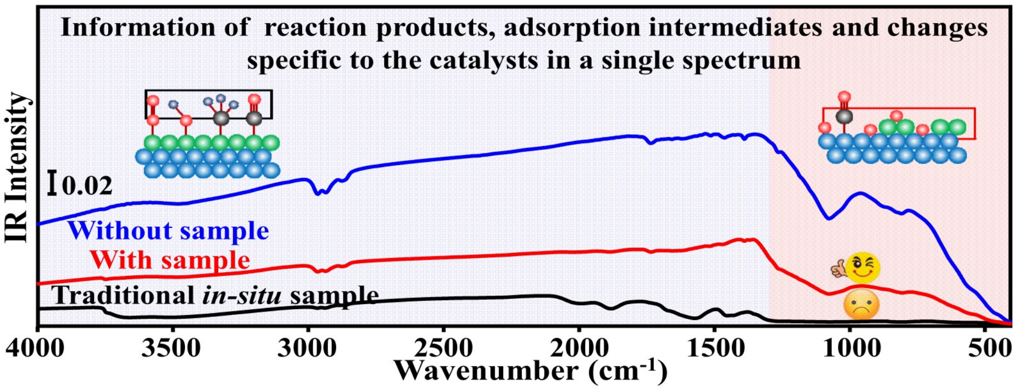


This review summarizes the recent progress in alkyne selective hydrogenation on Pd-based catalysts, especially the understanding of the relationship between catalyst surface structure and catalytic selectivity, as demonstrated by surface science experiments and theoretical simulations.

Chin. J. Catal., 2022, 43: 2001–2009 doi: 10.1016/S1872-2067(21)64054-8 **[Article]**

Applications of *in-situ* wide spectral range infrared absorption spectroscopy for CO oxidation over Pd/SiO_2 and Cu/SiO_2 catalysts

Xuefei Weng, Shuangli Yang, Ding Ding, Mingshu Chen *, Huilin Wan
Xiamen University

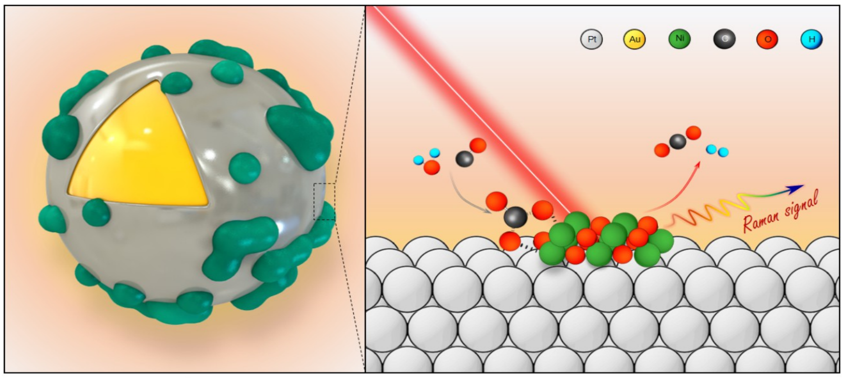


Surface adsorption intermediates and changes of the catalysts, as well as the formation products can be obtained in a single IR spectrum under reaction condition.

Chin. J. Catal., 2022, 43: 2010–2016 doi: 10.1016/S1872-2067(21)63964-5 **[Article]**

Direct identification of the carbonate intermediate during water-gas shift reaction at Pt-NiO interfaces using surface-enhanced Raman spectroscopy

Si-Na Qin, Di-Ye Wei, Jie Wei, Jia-Sheng Lin, Qing-Qi Chen, Yuan-Fei Wu, Huai-Zhou Jin *, Hua Zhang *, Jian-Feng Li *
Xiamen University; China Jiliang University

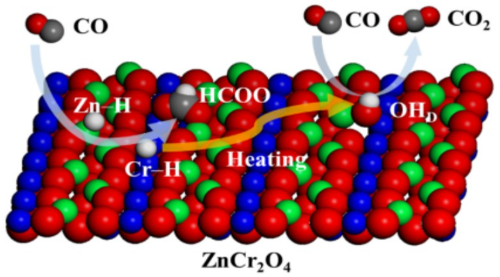


Direct spectroscopic evidence of the carbonate intermediate and its evolution during water-gas shift reaction at Pt-NiO interfaces is obtained using surface-enhanced Raman spectroscopy, based on which the reaction mechanism is then proposed.

Chin. J. Catal., 2022, 43: 2017–2025 doi: 10.1016/S1872-2067(21)64008-1 **[Article]**

Probing active species for CO hydrogenation over ZnCr$_2$O$_4$ catalysts

Yunjian Ling, Yihua Ran, Weipeng Shao, Na Li, Feng Jiao, Xiulian Pan, Qiang Fu, Zhi Liu, Fan Yang *, Xinhe Bao
Dalian Institute of Chemical Physics; Chinese Academy of Sciences; ShanghaiTech University

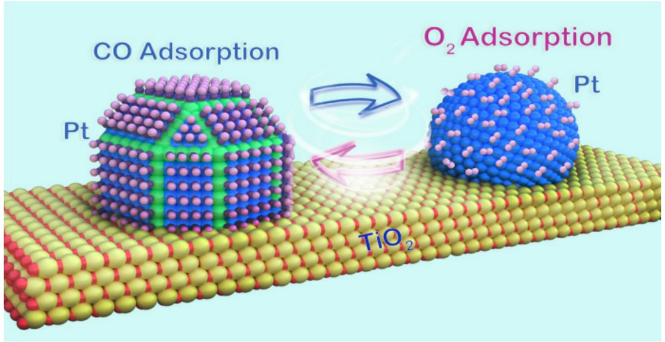


Surface hydroxyl species are consumed by CO *via* the route of water-gas-shift reaction, while surface hydride species would hydrogenate CO to form formate. Surface hydride species could transform into hydroxyl species on ZnCr$_2$O$_4$ at elevated temperatures.

Chin. J. Catal., 2022, 43: 2026–2033 doi: 10.1016/S1872-2067(21)63958-X **[Article]**

Reversible transformation between terrace and step sites of Pt nanoparticles on titanium under CO and O$_2$ environments

Yang Ou, Songda Li, Fei Wang, Xinyi Duan, Wentao Yuan *, Hangsheng Yang, Ze Zhang, Yong Wang *
Zhejiang University;
Shanghai Institute of Applied Physics;
University of Chinese Academy of Science

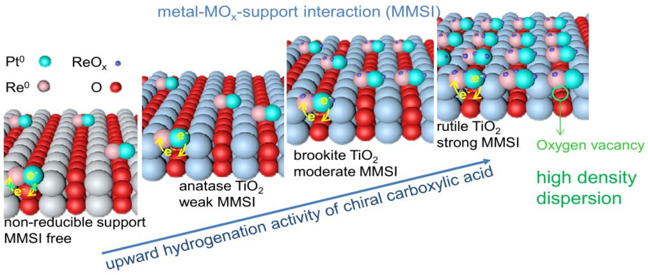


A reversible surface structural transformation between terrace and step sites of Pt catalysts under CO and O$_2$ environments was revealed, *via in situ* atmospheric transmission electron microscopy and *in situ* Fourier transform infrared spectroscopy.

Chin. J. Catal., 2022, 43: 2034–2044 doi: 10.1016/S1872-2067(21)64021-4 **[Article]**

Boosting chiral carboxylic acid hydrogenation by tuning metal-MO$_x$-support interaction in PtReO$_x$/TiO$_2$ catalysts

Guang Gao, Zelun Zhao, Jia Wang, Yongjie Xi, Peng Sun *, Fuwei Li *
Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences



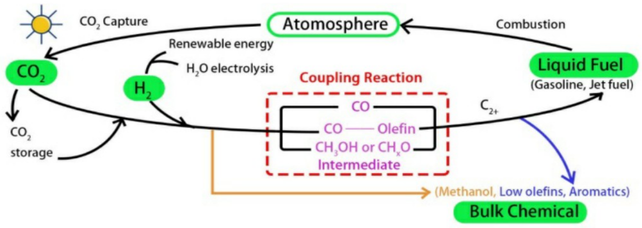
TiO$_2$-crystalline-phase-dependent density of oxygen vacancies induces the formation of different Pt-ReO$_x$-TiO$_2$ interaction, which dominates the electron transfer therein and tunes the adsorption strength of carbonyl moiety of carboxylic acid, and thus promoting hydrogenation activity and selectivity.

Account

Chin. J. Catal., 2022, 43: 2045–2056 doi: 10.1016/S1872-2067(22)64107-X

Direct carbon dioxide hydrogenation to produce bulk chemicals and liquid fuels *via* heterogeneous catalysis

Zixuan Zhou, Peng Gao *
Shanghai Advanced Research Institute, Chinese Academy of Sciences; University of the Chinese Academy of Sciences



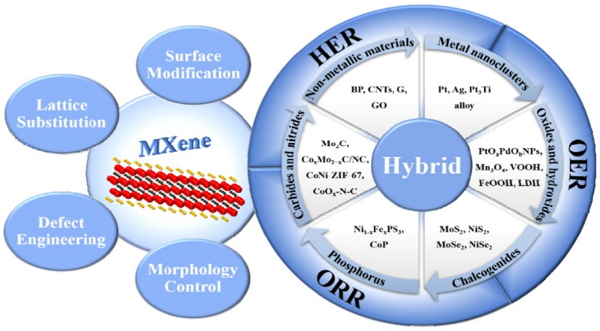
The hydrogenation of CO$_2$ to chemicals and fuels has a distinct CO$_2$ emission reduction effect. In this study, the catalyst design, selectivity regulation, structure-performance relationship, and reaction mechanism are discussed in detail.

Reviews

Chin. J. Catal., 2022, 43: 2057–2090 doi: 10.1016/S1872-2067(21)64030-5

MXenes for electrocatalysis applications: Modification and hybridization

Xue Bai, Jingqi Guan *
Jilin University

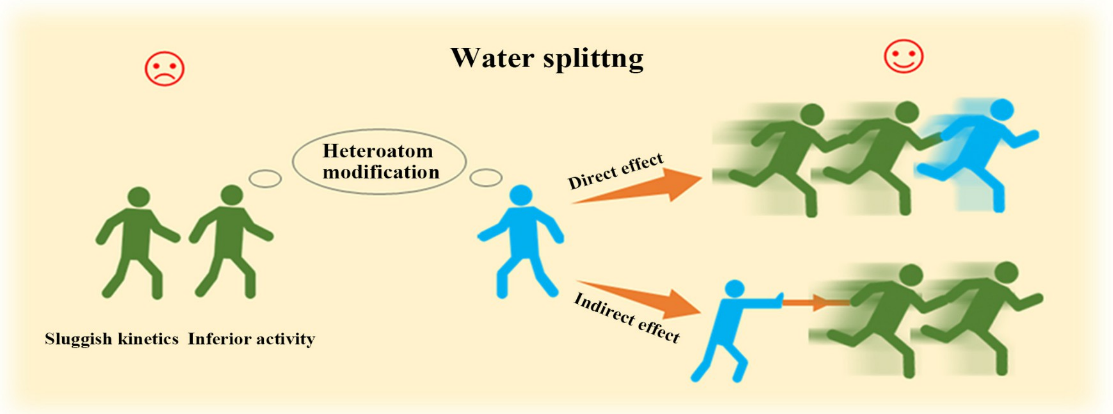


This review summarizes the progress of MXene-based electrocatalysts for the HER, OER, and ORR, including regulating pristine MXenes and modifying hybrid MXenes, from both theoretical and experimental perspectives.

Chin. J. Catal., 2022, 43: 2091–2110 doi: 10.1016/S1872-2067(21)64052-4

Roles of heteroatoms in electrocatalysts for alkaline water splitting: A review focusing on the reaction mechanism

Chuqiang Huang, Jianqing Zhou, Dingshuo Duan, Qiancheng Zhou, Jieming Wang, Bowen Peng, Luo Yu *, Ying Yu *
Central China Normal University; The Chinese University of Hong Kong; Hubei Normal University

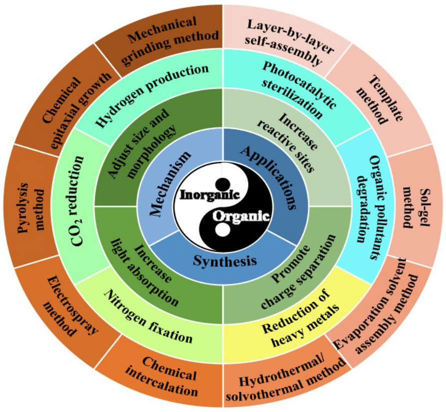


This review provides a summary and perspective on the key roles of heteroatoms for the improved reaction kinetics of alkaline water splitting based on reaction pathways.

Chin. J. Catal., 2022, 43: 2111–2140 doi: 10.1016/S1872-2067(22)64096-8

Inorganic-organic hybrid photocatalysts: Syntheses, mechanisms, and applications

Hui Yang, Kai Dai *, Jinfeng Zhang *, Graham Dawson
Huaibei Normal University; Xi'an Jiaotong Liverpool University

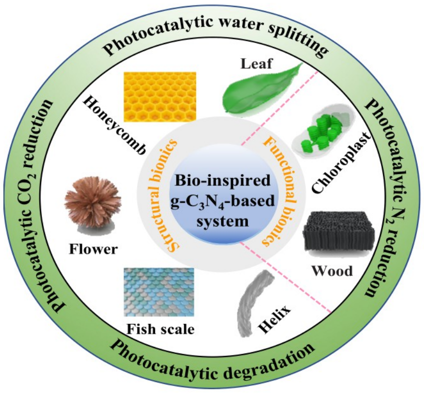


In this paper, the design principles and synthesis strategies of inorganic–organic hybrid materials are reviewed and their functions and mechanisms are described. Finally, the application of inorganic–organic hybrid materials in photocatalysis is introduced.

Chin. J. Catal., 2022, 43: 2141–2172 doi: 10.1016/S1872-2067(22)64110-X

Bio-inspired nanostructured g-C_3N_4-based photocatalysts: A comprehensive review

Bo Lin, Mengyang Xia, Baorong Xu, Ben Chong, Zihao Chen, Guidong Yang *
Xi'an Jiaotong University



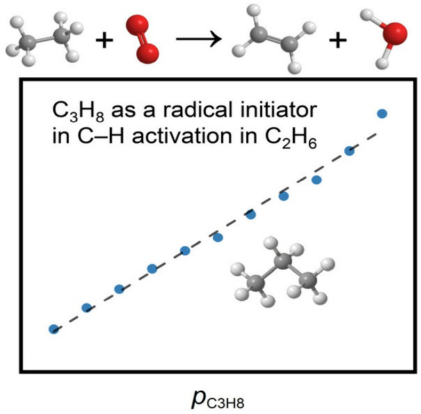
This review summarizes the fundamentals and recent advances of bio-inspired structured g-C_3N_4-based photocatalysts, which aims to expand the knowledge on bio-inspired nanostructured g-C_3N_4-based photocatalysts, thus advancing the development of biomimetic photocatalysis.

Articles

Chin. J. Catal., 2022, 43: 2173–2182 doi: 10.1016/S1872-2067(21)64042-1

Oxidative co-dehydrogenation of ethane and propane over h-BN as an effective means for C–H bond activation and mechanistic investigations

Hao Tian, Bingjun Xu *
Peking University

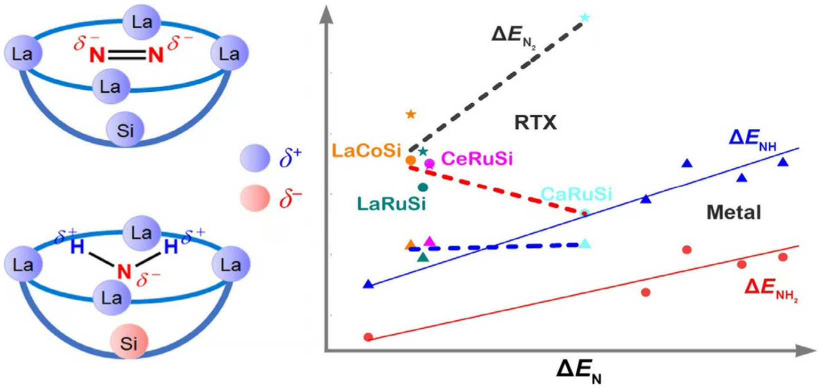


In oxidative dehydrogenation of mixed alkanes catalyzed by hexagonal boron nitride, ethane conversion rates exhibit a first order kinetics toward the partial pressure of propane, indicating a radical chain mechanism with shared H-abstractor.

Chin. J. Catal., 2022, 43: 2183–2192 doi: 10.1016/S1872-2067(22)64129-9

Breaking the scaling relations for efficient N_2-to-NH_3 conversion by a bowl active site design: Insight from LaRuSi and isostructural electrides

Ya-Fei Jiang, Jin-Cheng Liu, Cong-Qiao Xu, Jun Li, Hai Xiao *
Tsinghua University; Southern University of Science and Technology

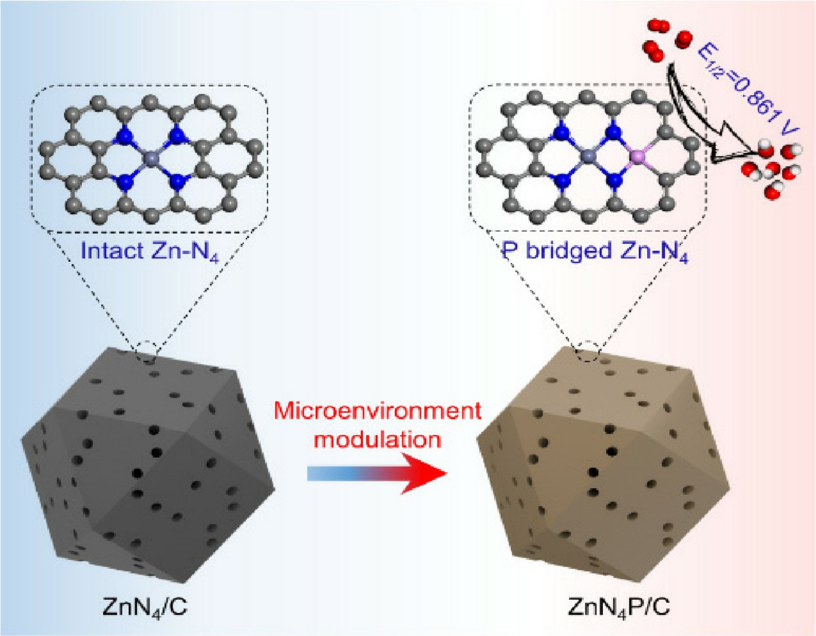


A bowl active site on the lanthanide intermetallic electride LaRuSi, composed of four surface La cations and one subsurface Si atom, plays the key role in efficient catalysis of N_2-to-NH_3 conversion by breaking the scaling relations through specific electrostatic and orbital interactions. This bowl active site thus presents a design concept of highly efficient heterogeneous catalyst for N_2-to-NH_3 conversion.

Chin. J. Catal., 2022, 43: 2193–2201 doi: 10.1016/S1872-2067(22)64089-0

Modulating the microenvironment structure of single Zn atom: ZnN_4P/C active site for boosted oxygen reduction reaction

Syed Shoaib Ahmad Shah, Tayyaba Najam *, Jiao Yang, Muhammad Sufyan Javed, Lishan Peng *, Zidong Wei *
Chongqing University, China; Southwest University, China; Shenzhen University, China; Lanzhou University, China;
The University of Auckland, New Zealand; Ganjiang Innovation Academy, Chinese Academy of Sciences, China



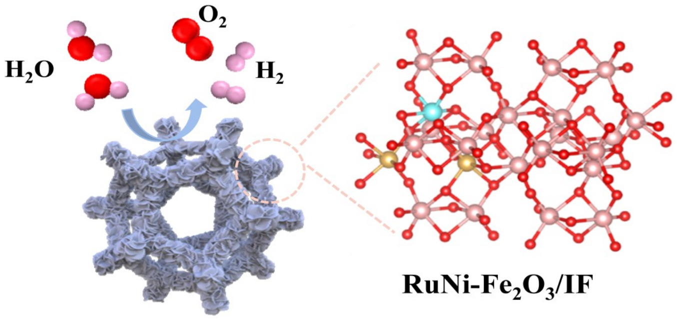
The microenvironment modulation of Zn single atom catalysts by P-doping enhanced the catalytic performance of single atoms for ORR and Zn-air battery by altering the electronic structure of central metal atom.

Chin. J. Catal., 2022, 43: 2202–2211 doi: 10.1016/S1872-2067(22)64093-2

Controllable synthesis of a self-assembled ultralow Ru, Ni-doped Fe_2O_3 lily as a bifunctional electrocatalyst for large-current-density alkaline seawater electrolysis

Tong Cui, Xuejun Zhai, Lili Guo, Jing-Qi Chi *, Yu Zhang, Jiawei Zhu, Xuemei Sun, Lei Wang *
Qingdao University of Science and Technology

A self-assembled ultralow Ru, Ni-doped Fe_2O_3 (RuNi-Fe_2O_3/IF) catalyst with a lily-shaped morphology grown on iron foam was synthesized using a controllable hydrothermal method. Benefitting from the Ru/Ni chemical substitution, RuNi-Fe_2O_3/IF possesses benchmark electrocatalytic activity and stability toward HER and OER in 1.0 mol L^{-1} KOH and 1.0 mol L^{-1} KOH seawater electrolytes.

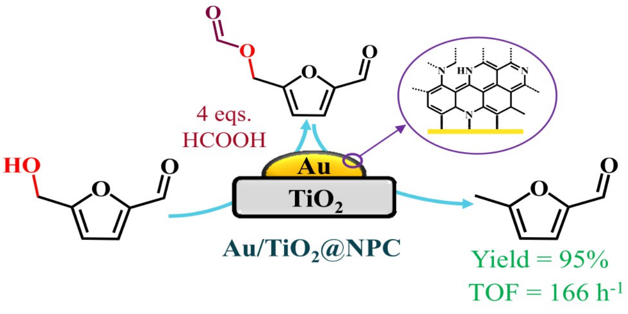


Chin. J. Catal., 2022, 43: 2212–2222 doi: 10.1016/S1872-2067(21)64049-4

N-doped carbon layer-coated Au nanocatalyst for H_2-free conversion of 5-hydroxymethylfurfural to 5-methylfurfural

Jiang Zhang, Zijian Wang, Mugeng Chen, Yifeng Zhu, Yongmei Liu, Heyong He, Yong Cao *, Xinhe Bao *
Fudan University;
Dalian Institute of Chemical Physics, Chinese Academy of Sciences

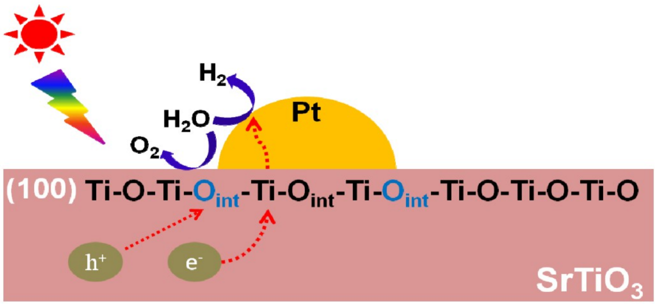
N-doped carbon layer-coated Au nanocatalyst provided high yield in the chemoselective transformation of HMF into 5-MF using only 4 equivalents of HCOOH as the deoxygenation reagent. The unique catalyst also showed high HCOOH utilization efficiency.



Chin. J. Catal., 2022, 43: 2223–2230 doi: 10.1016/S1872-2067(21)64048-2

Water oxidation sites located at the interface of Pt/$SrTiO_3$ for photocatalytic overall water splitting

Xianwen Zhang, Zheng Li, Taifeng Liu, Mingrun Li, Chaobin Zeng, Hiroaki Matsumoto, Hongxian Han *
Dalian Institute of Chemical Physics, Chinese Academy of Sciences; University of Chinese Academy of Sciences; Henan University; Hitachi High-Tech (Shanghai) Co., Ltd.

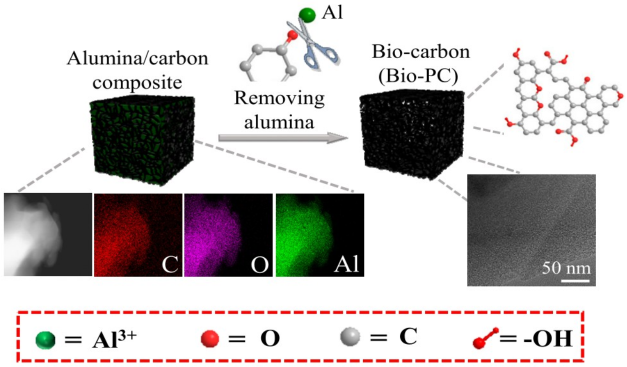


During photocatalytic overall water splitting, the active sites for water oxidation are mainly located at the interface between Pt cocatalyst and $SrTiO_3$ photocatalyst.

Chin. J. Catal., 2022, 43: 2231–2239 doi: 10.1016/S1872-2067(21)64031-7

Interfacial-interaction-induced fabrication of biomass-derived porous carbon with enhanced intrinsic active sites

Wenjuan Zhang, Pei Jing, Juan Du, Shujie Wu, Wenfu Yan, Gang Liu *
Jilin University; Jilin Normal University

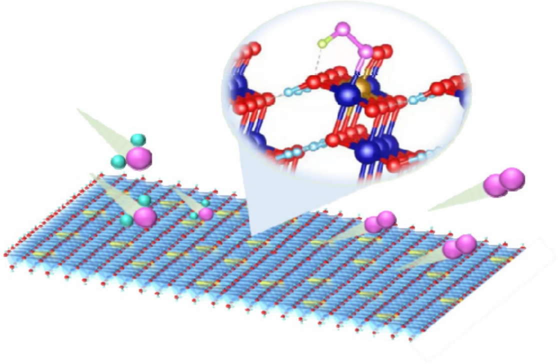


Under non-oxidation conditions, *in-situ* formed alumina/carbon interface was developed as a cradle for the generation of accessible active sites. It can also tune the porous structure of resultant carbon in the micro- and meso-range.

Chin. J. Catal., 2022, 43: 2240–2248 doi: 10.1016/S1872-2067(21)64033-0

Unveiling the active sites of ultrathin Co-Fe layered double hydroxides for the oxygen evolution reaction

Xue Bai, Zhiyao Duan *, Bing Nan, Liming Wang, Tianmi Tang, Jingqi Guan *
Jilin University; Northwestern Polytechnical University; Shanghai Advanced Research Institute, Chinese Academy of Science; Institute of High Energy Physics, Chinese Academy of Sciences;



Ultrathin CoFe LDH displays a low overpotential (256 mV) at 10 mA cm^{-2}. The surface Co sites adjacent to Fe atoms are the active centers for the OER.

Chin. J. Catal., 2022, 43: 2249–2258 doi: 10.1016/S1872-2067(22)64109-3

Direct Z-scheme photochemical hybrid systems: Loading porphyrin-based metal-organic cages on graphitic-C_3N_4 to dramatically enhance photocatalytic hydrogen evolution

Yang Lei, Jian-Feng Huang, Xin-Ao Li, Chu-Ying Lv, Chao-Ping Hou, Jun-Min Liu *
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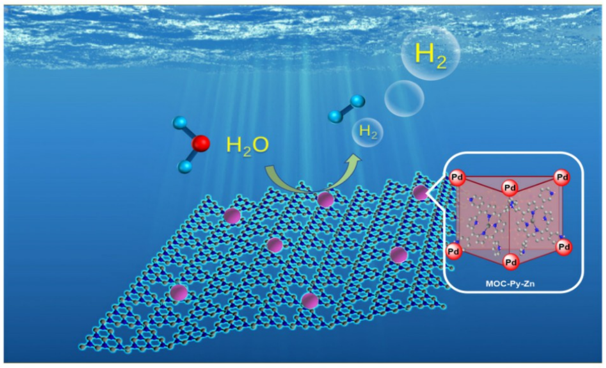

A direct Z-scheme photochemical hybrid system MOC-Py-Zn/g-C_3N_4 is constructed for the first time by immobilizing porphyrin-based metal-organic cages on graphitic-C_3N_4, and used for efficient and stable photocatalytic hydrogen evolution from water.

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Conversion of methanol to propylene over SAPO-14: Reaction mechanism and catalyst deactivation

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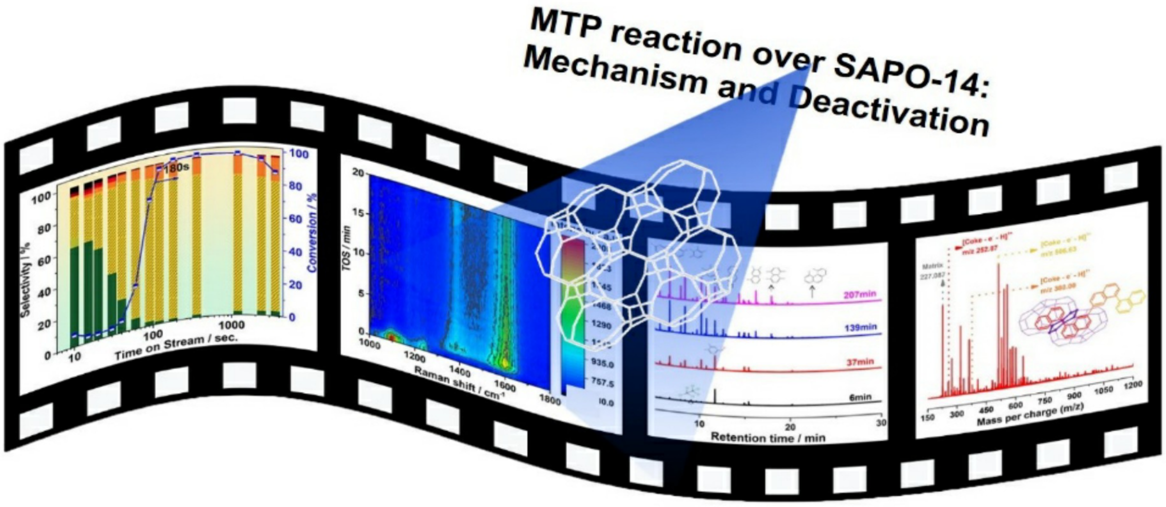

The reaction mechanism and deactivation process of methanol-to-propylene conversion over SAPO-14 were investigated through various *in situ* and *ex situ* techniques, revealing the evolution of the reaction pathway from a dual cycle to an olefins-based cycle.