Chinese Journal of Catalysis

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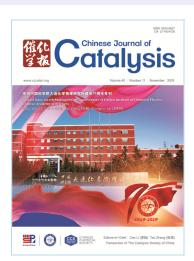








In This Issue



Cover: The year 2019 marks the 70th anniversary of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences (abbreviated as DICP). Since its foundation, DICP has been at the forefront of fundamental and applied sciences and technologies that closely response the scientific and economic demands of China. After the efforts of several generations, DICP has gained a high reputation in chemistry research, covering from fundamental studies, technology development to industrial applications. Especially, DICP has made great contributions in the field of catalysis. To celebrate the 70th anniversary, the journal publishes this special issue. Internationally renowned catalysis scientists were kindly invited to make contributions. The speical issue contains 23 papers, including 2 Editorials, 3 Reviews, 1 Communication, and 17 research Articles that cover aspects of both fundamental studies and industrial applications.

對面: 2019 年是中国科学院大连化学物理研究所(简称大连化物所)建所70 周年. 大连化物所是一个基础研究与应用研究并重、应用研究和技术转化相结合,以任务带学科为主要特色的综合性研究所. 七十年来,研究所不断积累和调整,逐步在催化化学、工程化学、化学激光、分子反应动力学、分析化学和生物技术等领域形成了特色. 特别是在催化化学领域取得了一系列重大科技成果,为科学技术发展做出了重要的贡献. 本期庆祝大连化物所建所 70 周年专刊共邀请国际催化领域权威专家的 23 篇文章,包括 2 篇回顾、3 篇综述、1 篇快讯和 17 篇论文,展示了国际国内催化领域的研究进展及大连化物所在催化领域所取得的成就.

About the Journal

Chinese Journal of Catalysis is an international journal published monthly by Chinese Chemical Society, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and Elsevier. The journal publishes original, rigorous, and scholarly contributions in the fields of heterogeneous and homogeneous catalysis in English or in both English and Chinese. The scope of the journal includes:

- New trends in catalysis for applications in energy production, environmental protection, and production of new materials, petroleum chemicals, and fine chemicals;
- Scientific foundation for the preparation and activation of catalysts of commercial interest or their representative models;
- Spectroscopic methods for structural characterization, especially methods for in situ characterization;
- New theoretical methods of potential practical interest and impact in the science and applications of catalysis and catalytic reaction;
- Relationship between homogeneous and heterogeneous catalysis;
- Theoretical studies on the structure and reactivity of catalysts.
- The journal also accepts contributions dealing with photo-catalysis, bio-catalysis, and surface science and chemical kinetics issues
 related to catalysis.

Types of Contributions

- Reviews deal with topics of current interest in the areas covered by this journal. Reviews are surveys, with entire, systematic, and important information, of recent progress in important topics of catalysis. Rather than an assemblage of detailed information or a complete literature survey, a critically selected treatment of the material is desired. Unsolved problems and possible developments should also be discussed. Authors should have published articles in the field. Reviews should have more than 80 references.
- *Communications* rapidly report studies with significant innovation and major academic value. They are limited to four Journal pages. After publication, their full-text papers can also be submitted to this or other journals.
- Articles are original full-text reports on innovative, systematic and completed research on catalysis.
- Highlights describe and comment on very important new results in the original
 research of a third person with a view to highlight their significance. The results should
 be presented clearly and concisely without the comprehensive details required for an
 original article.
- Perspectives are short reviews of recent developments in an established or developing topical field. The authors should offer a critical assessment of the trend of the field, rather than a summary of literatures.
- Viewpoints describe the results of original research in general in some area, with a view
 to highlighting the progress, analyzing the major problems, and commenting the
 possible research target and direction in the future.

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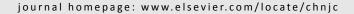
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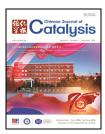
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Special Issue on Celebrating the 70th Anniversary of Dalian Institute of Chemical Physics, Chinese Academy of Sciences

Guest Editors: Can Li, Tao Zhang, Zhongmin Liu

Chinese Journal of Catalysis

Graphical Contents

Editorials

Chin. J. Catal., 2019, 40: 1589–1590 doi: S1872-2067(19)63457-1

Preface to Special Issue on Celebrating the 70th Anniversary of Dalian Institute of Chemical Physics, Chinese Academy of Sciences

Can Li, Tao Zhang, Zhongmin Liu

Dalian Institute of Chemical Physics, CAS; Chinese Academy of Sciences, China







Chin. J. Catal., 2019, 40: 1591-1614 doi: \$1872-2067(19)63483-2

History of the Dalian Institute of Chemical Physics and the friendship between China and Japan in catalysis

S. Ted Oyama * with Qin Xin, Guoxing Xiong, Wenjie Shen, Jie Xu, Hongmei Yin, Youzhu Yuan, Haichao Liu, Huidong Zheng Fuzhou University, China; The University of Tokyo, Japan; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China; Xiamen University, China; Peking University, China



The year 2019 marks the 70^{th} anniversary of the beginning of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences (DICP). This article presents a history of the origins of DICP and relates the recent friendship between China and Japan in the field of catalysis.

Chin. J. Catal., 2019, 40: 1615–1626 doi: \$1872-2067(19)63482-0

An odyssey: The Way Chinese catalysis towards the world

Qin Xin *, Yongxue Li Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China; University of Liverpool, UK

With the careful planning and arrangements by the Chinese catalytic elites, the quadrennial grand event in the international catalytic world—the 16^{th} International Congress on Catalysis (ICC) was successively held in Beijing presentations indicating the frontiers of the catalytic science and the magnanimity of the organizers. This paper reviewed the development of catalytic science and technology of China from scratch to small then to large under the efforts of several generations.

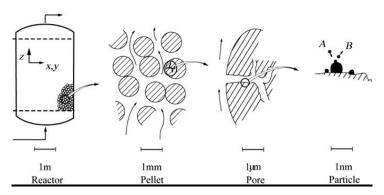


Reviews

Chin. J. Catal., 2019, 40: 1627-1636 doi: 10.1016/S1872-2067(18)63162-6

Importance, features and uses of metal oxide catalysts in heterogeneous catalysis

Jacques C. Védrine *
Sorbonne Université, France



This review aims at assembling the present state of the art of the multiuses of metal oxides in heterogeneous catalysis, concerning liquid and gaseous phases of the reactant mixtures on solid catalysts.

Chin. J. Catal., 2019, 40: 1637–1654 doi: \$1872-2067(19)63372-3

Advanced characterization for industrial catalysis applications

Shelly Kelly *, Wharton Sinkler *, Lijun Xu, Sergio Sanchez, Cem Akatay, Haiyan Wang, John Qianjun Chen Honeywell UOP, USA

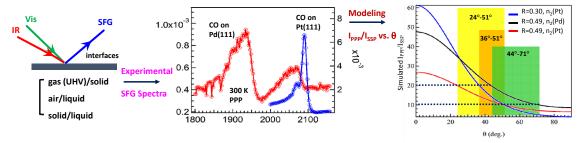


Surface and bulk chemistry characterization is reviewed for two major catalytic functions: Supported Pt nano-clusters and layered Group VI sulfides. Trends are identified relating structure with catalytic activity, and areas for improvement.

Chin. J. Catal., 2019, 40: 1655-1667 doi: S1872-2067(19)63357-7

A modeling analysis of molecular orientation at interfaces by polarization-dependent sum frequency generation vibrational spectroscopy

Xia Li, Günther Rupprechter * Technische Universität Wien, Austria



Even slight changes of refractive index (medium 2) and hyperpolarizability ratio ($R = \beta aac/\beta ccc$), which are usually rather ignored, have significant effects on the SFG spectral intensity and molecular orientation of gas (UHV)/solid, air/liquid and solid/liquid interfaces.

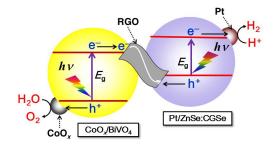
Communication

Chin. J. Catal., 2019, 40: 1668–1672 doi: \$1872-2067(19)63326-7

Metal selenides for photocatalytic Z-scheme pure water splitting mediated by reduced graphene oxide

Shanshan Chen, Takashi Hisatomi, Guijun Ma, Zheng Wang, Zhenhua Pan, Tsuyoshi Takata, Kazunari Domen * Shinshu University, Japan; The University of Tokyo, Japan

Powder suspension Z-scheme pure water splitting systems employing narrow bandgap metal selenides, $CoO_x/BiVO_4$, and reduced graphene oxide as the H_2 evolving photocatalyst, O_2 evolving photocatalyst, and electron mediator, respectively, are demonstrated.



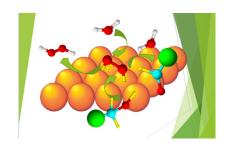
Articles

Chin. J. Catal., 2019, 40: 1673-1678 doi: \$1872-2067(19)63327-9

Prospect of vapor phase catalytic H_2O_2 production by oxidation of water

Mayfair C. Kung, Harold H. Kung * Northwestern University, USA

Efficient coupling of some catalytic organic oxidation reactions with oxidation of water by molecular oxygen enables production of hydrogen peroxide.



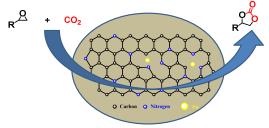
Chin. J. Catal., 2019, 40: 1679-1685 doi: S1872-2067(19)63316-4

Zinc single atoms on N-doped carbon: An efficient and stable catalyst for CO_2 fixation and conversion

Xinjiang Cui, Xingchao Dai, Annette-Enrica Surkus, Kathrin Junge, Carsten Kreyenschulte, Giovanni Agostini, Nils Rockstroh, Matthias Beller*

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

A novel Zn single atom catalyst (Zn-SAC) supported on N-doped carbon material was prepared. The resulting catalyst allows for efficient and general activation of functionalized terminal epoxides to give the corresponding carbonates in high yields.



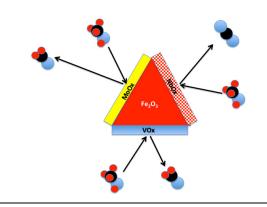
Single Atom Catalyst

Chin. J. Catal., 2019, 40: 1686-1692 doi: \$1872-2067(19)63350-4

Methanol oxidation over shell-core MO_x/Fe_2O_3 (M = Mo, V, Nb) catalysts

Pip Hellier, Peter P. Wells, Michael Bowker *
UK Catalysis Hub, UK; Cardiff University, UK; University of Southampton,
UK; Diamond Light Source Ltd, UK

Methanol oxidation on three surface oxides on Fe_2O_3 showing the main carbon products. Mo and V monolayers are selective to formal-dehyde, while Nb does not make complete monolayers and mainly combusts to CO_2 .

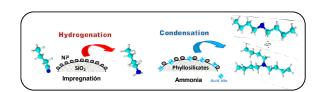


Chin. J. Catal., 2019, 40: 1693-1703 doi: 10.1016/S1872-2067(18)63179-1

Effect of the catalyst preparation method on the performance of Ni-supported catalysts for the synthesis of saturated amines from nitrile hydrogenation

D. J. Segobia, A. F. Trasarti, C. R. Apesteguía * INCAPE, UNL-CONICET, CCT Conicet- Paraje El Pozo, Argentina

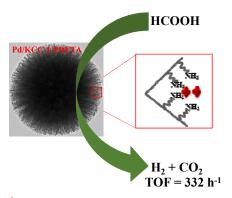
 Ni/SiO_2 prepared by the ammonia method forms selectively secondary and tertiary amines from butyronitrile hydrogenation. The catalyst contains Ni^0 nanoparticles in close contact with Ni^{*2} species in Ni phyllosilicates that favor the condensation reactions.



Chin. J. Catal., 2019, 40: 1704-1712 doi: S1872-2067(19)63303-6

Catalytic dehydrogenation of formic acid over palladium nanoparticles immobilized on fibrous mesoporous silica KCC-1

Siqian Zhang, Yingjie Qian, Wha-Seung Ahn* Inha University, Republic of Korea



Highly efficient dehydrogenation of formic acid without any additives at 323 K was achieved using Pd nanoparticles supported on amine-functionalized fibrous silica KCC-1.

♦ Pd (nanoparticle size=2.75 nm)

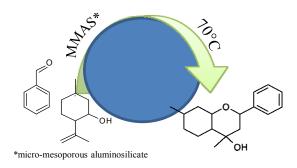
The N-(3-trimethoxysilylpropyl) diethylenetriamine (PDETA)

Chin. J. Catal., 2019, 40: 1713-1720 doi: S1872-2067(19)63305-X

Prins cyclisation of (-)-isopulegol with benzaldehyde over ZSM-5 based micro-mesoporous catalysts for production of pharmaceuticals

Ekaterina Kholkina, Päivi Mäki-Arvela, Chloe Lozachmeuer, Roman Barakov, Nataliya Shcherban, Dmitry Yu. Murzin Åbo Akademi University, Finland; National Academy of Sciences of Ukraine, Ukraine

Strongly acidic MMAS catalysts were beneficial in Prins cyclisation for production of biologically active 2H-chromene derivatives.



Chin. J. Catal., 2019, 40: 1721-1730 doi: S1872-2067(19)63345-0

Hydrodeoxygenation of anisole over different Rh surfaces

Nhung N. Duong, Darius Aruho, Bin Wang*, Daniel E. Resasco* University of Oklahoma, USA; Vietnam National University, Vietnam

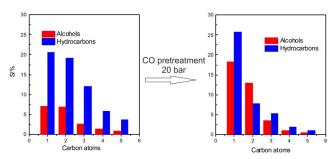


Manipulating the surface coordination of rhodium atoms can greatly affect the metal oxophilicity and in turn control its activity for C–O bond cleavage. In the hydrodeoxygenation of anisole, a step surface favors deoxygenation to benzene while a smooth terrace prefers hydrogenation to phenol.

Chin. J. Catal., 2019, 40: 1731-1740 doi: S1872-2067(19)63344-9

On the role of cobalt carbidization in higher alcohol synthesis over hydrotalcite-based Co-Cu catalysts

Janine Nebel, Stefan Schmidt, Qiushi Pan, Katrin Lotz, Stefan Kaluza*, Martin Muhler*
Ruhr-University Bochum, Germany; Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT, Germany

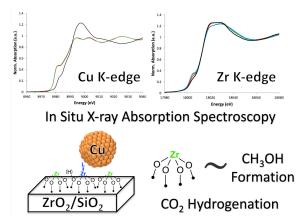


CO pretreatment at elevated pressure enhances the selectivities to linear alcohols through surface cobalt enrichment and carbide formation.

Chin. J. Catal., 2019, 40: 1741-1748 doi: S1872-2067(19)63348-6

Zr(IV) surface sites determine CH₃OH formation rate on Cu/ZrO₂/SiO₂ - CO₂ hydrogenation catalysts

Erwin Lam, Kim Larmier, Shohei Tada, Patrick Wolf, Olga V. Safonova, Christophe Copéret *
ETH Zürich, Switzerland; Paul Scherrer Institute, Switzerland; IFP Energies Nouvelles, Rond-Point de l'échangeur de Solaize, France;
The University of Tokyo, Japan

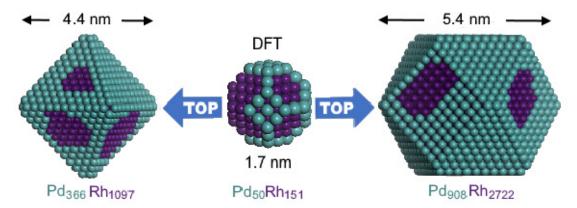


Density and role of Lewis acidic Zr(IV) surface sites in $Cu/SiO_2/ZrO_2$ based catalyst to promote CO_2 -to- CH_3OH synthesis is elucidated by in-situ X-ray absorption spectroscopy.

Chin. J. Catal., 2019, 40: 1749–1757 doi: S1872-2067(19)63362-0

Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications

Lorena Vega, Hristiyan A. Aleksandrov *, Konstantin M. Neyman *
University of Barcelona, Spain; University of Sofia, Bulgaria; Catalan Institution for Research and Advanced Studies (ICREA), Spain



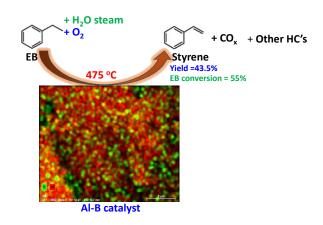
Catalytically active Pd-Rh nanoparticles adapt their surface to chemical environment. Density functional modelling identifies surface composition of Pd-Rh particles containing thousands atoms and paves the way for evaluating surface segregation caused by adsorbed reactants.

Chin. J. Catal., 2019, 40: 1758–1765 doi: S1872-2067(19)63432-7

Alumina-boron catalysts for oxidative dehydrogenation of ethylbenzene to styrene: Influence of alumina-boron composition and method of preparation on catalysts properties

Nagaraju Pasupulety*, Muhammad A. Daous, Abdulrahim A. Al-Zahrani, Hafedh Driss, Lachezar A. Petrov* King Abdulaziz University, Saudi Arabia

Boron addition to Al improved the acidity of the Al-B catalysts. Styrene formation depends on the nature of acid sites which were influenced by the Al-B catalyst method of preparation.

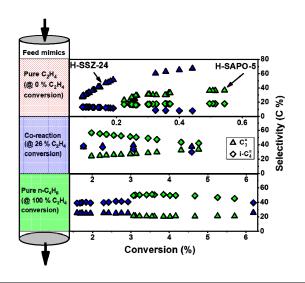


Chin. J. Catal., 2019, 40: 1766-1777 doi: S1872-2067(19)63426-1

Ethene and butene oligomerization over isostructural H-SAPO-5 and H-SSZ-24: Kinetics and mechanism

Christian Ahoba-Sam, Marius Westgård Erichsen, Unni Olsbye * University of Oslo, Norway

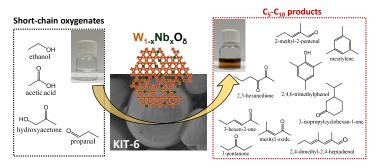
Reactor with three zones; representing the three measurement regimes. On the side; three typical conversion - selectivity graphs for H-SAPO-5 and H-SSZ-24, representing C3-C5 alkene selectivity in the three regimes.



Chin. J. Catal., 2019, 40: 1778-1787 doi: S1872-2067(19)63419-4

Reflux-synthesized bulk and diluted W-Nb-O mixed oxide bronzes for the valorization of short-chain oxygenates aqueous mixtures

D. Delgado, A. Fernández-Arroyo, N. La Salvia, M. E. Domine *, Jose M. López Nieto *
Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Spain



The incorporation of Nb into the h-WO₃ framework by a reflux method leads to a loss of periodicity in the ab plane of the crystal structure, with a concomitant increase of surface Lewis acidity; thus giving rise to higher yields to C_5 - C_{10} products in the valorization of aqueous model mixtures of short-chain oxygenates.

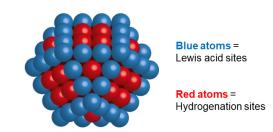
Chin. J. Catal., 2019, 40: 1788-1794 doi: S1872-2067(19)63392-9

Some insight on the structure/activity relationship of metal nanoparticles in Cu/SiO_2 catalysts

Nicola Scotti, Elisabetta Finocchio, Claudio Evangelisti, Marcello Marelli, Rinaldo Psaro, Nicoletta Ravasio *, Federica Zaccheria

CNR ISTM, Milano, Italy; University of Genoa, Genova, Italy

The activity of Cu/SiO_2 catalysts in the hydrogenation of 3-methyl-cyclohexanone was found to be linked to high coordination sites on the metal Cu particle, whereas acidic sites are represented by defective, low coordination sites.



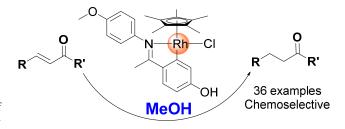
Chin. J. Catal., 2019, 40: 1795-1799 doi: S1872-2067(19)63367-X

Methanol as hydrogen source: Chemoselective transfer hydrogenation of α , β -unsaturated ketones with a rhodacycle

Ahmed H. Aboo, Robina Begum, Liangliang Zhao, Zahoor H. Farooqi, Jianliang Xiao *

University of Liverpool, United Kingdom; University of the Punjab, Pakistan

A rhodacycle catalyzes highly selective transfer hydrogenation of α,β -unsaturated ketones with MeOH as the source of hydrogen, affording saturated ketones exclusively.

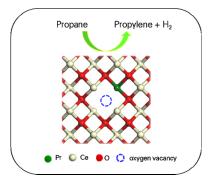


Chin. J. Catal., 2019, 40: 1800-1809 doi: \$1872-2067(19)63369-3

Activation of small molecules over praseodymium-doped ceria

Meiling Guo, Xuebin Liu, Angelo Amorelli * BP (China) Dalian Office, China; BP International, United Kingdom

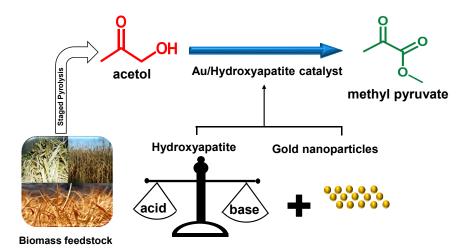
The praseodymium-doped ceria material in the absence of hydrogenation/dehydrogenation metals can selectively activate C–H bond of propane, giving a propylene selectivity of ca. 75% at a propane conversion of 5% to 10%.



Chin. J. Catal., 2019, 40: 1810-1819 doi: S1872-2067(19)63368-1

Oxidative esterification of acetol with methanol to methyl pyruvate over hydroxyapatite supported gold catalyst: Essential roles of acid-base properties

Yan Wan, Congcong Zheng, Xianchi Lei, Mengqi Zhuang, Jinhan Lin, Wenda Hu, Jingdong Lin, Shaolong Wan*, Yong Wang Xiamen University, China; Washington State University, USA



Au/hydroxyapatite (ratio of Ca/P = 1.62) catalyst exhibits superior performance toward the production of methyl pyruvate from biomass-derived acetol, where the featured acid-base properties in hydroxyapatite play an indispensable role.







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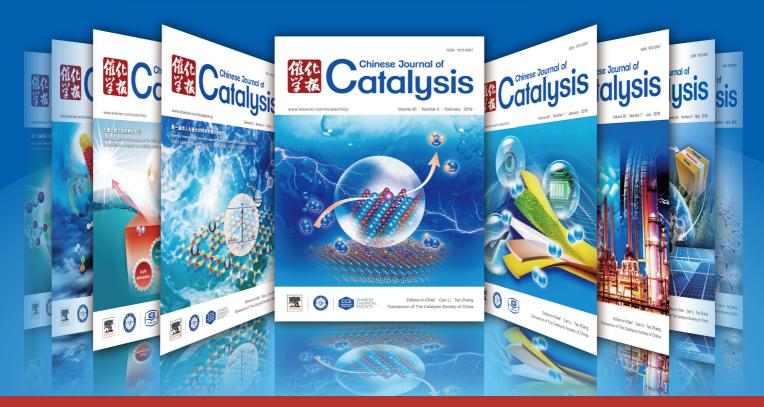
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