



# Chinese Journal of Catalysis

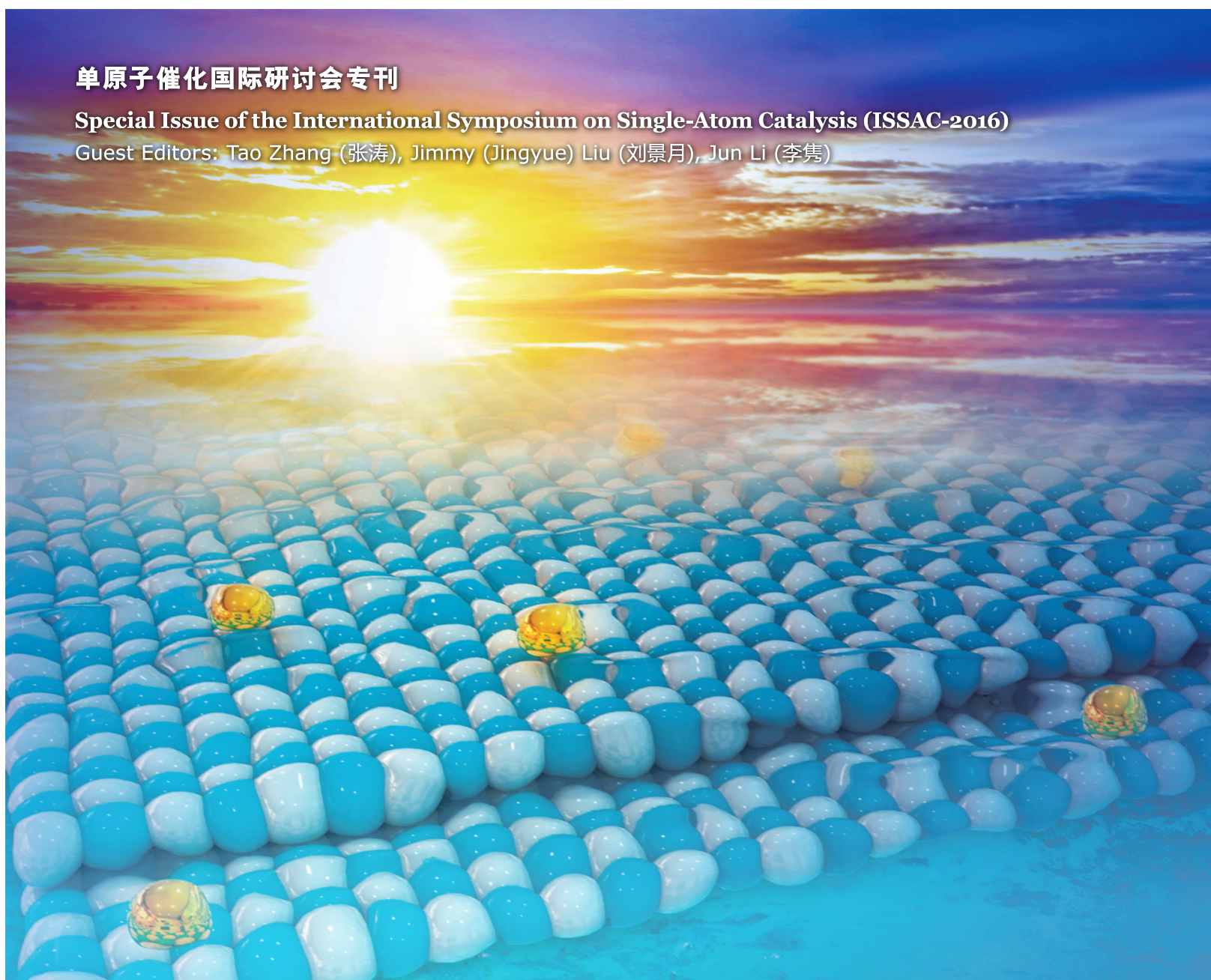
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Volume 38 | Number 9 | September 2017

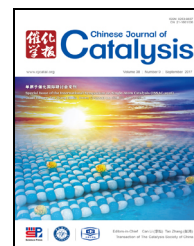
单原子催化国际研讨会专刊

Special Issue of the International Symposium on Single-Atom Catalysis (ISSAC-2016)

Guest Editors: Tao Zhang (张涛), Jimmy (Jingyue) Liu (刘景月), Jun Li (李隽)



Editors-in-Chief Can Li (李灿) Tao Zhang (张涛)  
Transaction of The Catalysis Society of China

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## Special Issue of the International Symposium on Single-Atom Catalysis (ISSAC-2016)

Guest Editors: Tao Zhang, Jimmy (Jingyue) Liu, Jun Li

### Chinese Journal of Catalysis

### Graphical Contents

#### Editorial

*Chin. J. Catal.*, 2017, 38: 1431 doi: 10.1016/S1872-2067(17)62895-X

#### Preface to the Special Issue of the International Symposium on Single-Atom Catalysis (ISSAC-2016)

Jun Li, Jimmy (Jingyue) Liu, Tao Zhang

*Tsinghua University, China; Arizona State University, United States; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*

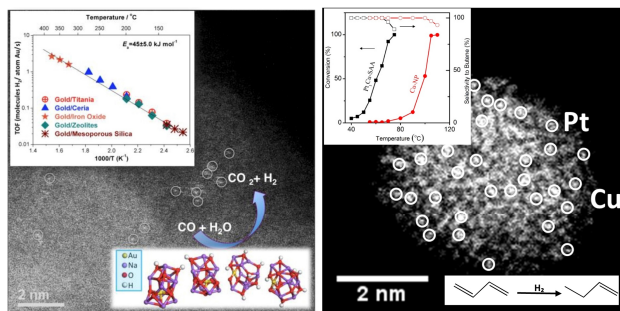


#### Viewpoint

*Chin. J. Catal.*, 2017, 38: 1432–1442 doi: 10.1016/S1872-2067(17)62886-9

#### Supported metal catalysts at the single-atom limit – A viewpoint

Maria Flytzani-Stephanopoulos\*  
*Tufts University, USA*



Single metal atoms supported on oxides catalyze the water-gas shift reaction. Single Atom Alloys (SAAs) comprise single metal atoms embedded in another metal surface. Shown here is the selective hydrogenation of butadiene to butene over PtCu SAAs at near ambient temperatures.

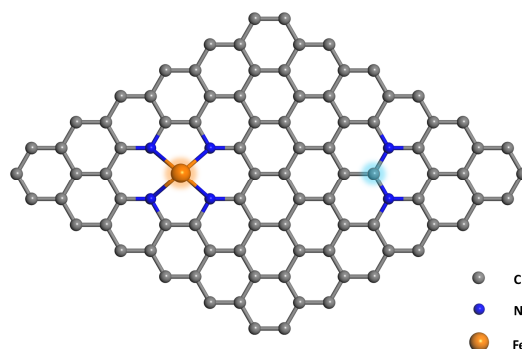
## Perspectives

*Chin. J. Catal.*, 2017, 38: 1443–1453 doi: 10.1016/S1872-2067(17)62839-0

### Two-dimensional materials confining single atoms for catalysis

Yong Wang, Wenhua Zhang, Dehui Deng \*, Xinhe Bao \*

*Dalian Institute of Chemical Physics, Chinese Academy of Sciences; Institute of Chemical Materials, China Academy of Engineering Physics; Xiamen University*



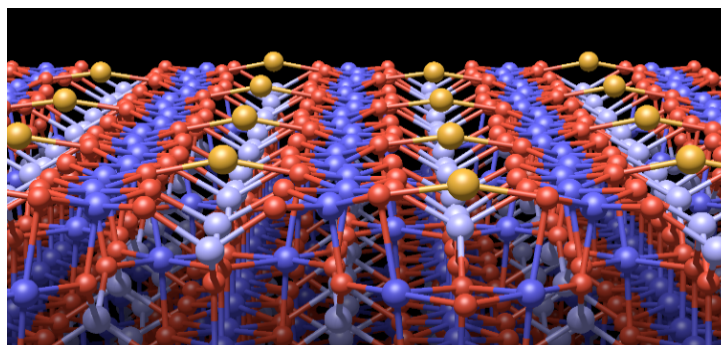
Two-dimensional materials confining single atoms, the mutually beneficial cooperation for highly efficient catalysis.

*Chin. J. Catal.*, 2017, 38: 1454–1459 doi: 10.1016/S1872-2067(17)62878-X

### Unravelling single atom catalysis: The surface science approach

Gareth S. Parkinson\*

*TU Wien, Austria*



This perspective discusses how studies of idealised model systems can shed light on the fundamental mechanisms of single-atom catalysis. The image shows Au adatoms supported by  $\text{Fe}_3\text{O}_4(001)$ .

*Chin. J. Catal.*, 2017, 38: 1460–1472 doi: 10.1016/S1872-2067(17)62900-0

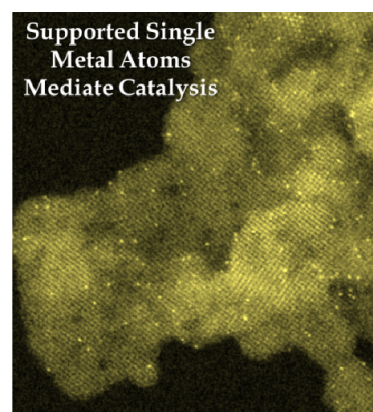
### Aberration-corrected scanning transmission electron microscopy in single-atom catalysis: Probing the catalytically active centers

Jingyue (Jimmy) Liu \*

*Arizona State University, United States;*

*Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*

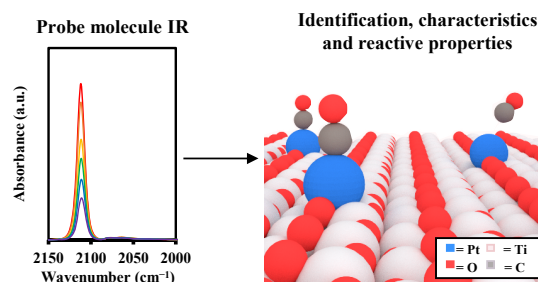
Aberration-corrected scanning transmission electron microscopy techniques are indispensable for understanding catalysis by supported single metal atoms and for developing practical single-atom catalysts for energy and chemical transformations.



*Chin. J. Catal.*, 2017, 38: 1473–1480 doi: 10.1016/S1872-2067(17)62882-1

### Using probe molecule FTIR spectroscopy to identify and characterize Pt-group metal based single atom catalysts

Chithra Asokan †, Leo DeRita †, Phillip Christopher \*  
University of California, USA

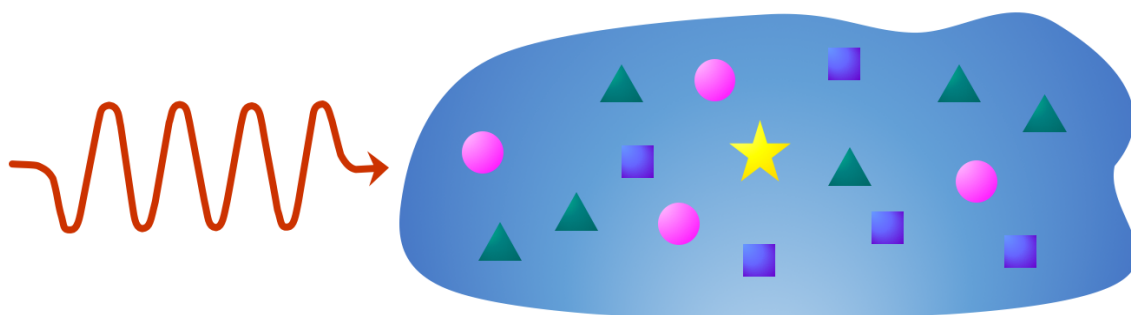


The utility, applications, and future directions of using probe molecule IR spectroscopy for identifying and characterizing catalysts consisting of supported Pt group metal single atom catalysts is presented in this perspective.

*Chin. J. Catal.*, 2017, 38: 1481–1488 doi: 10.1016/S1872-2067(17)62880-8

### X-ray absorption spectroscopy for single-atom catalysts: Critical importance and persistent challenges

Isao Ogino\*  
Hokkaido University, Japan

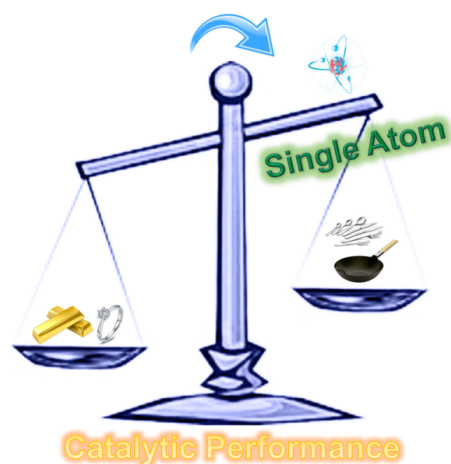


X-ray absorption spectroscopy is an essential technique to investigate the structure-performance relationship of single-atom catalysts. To benefit most from this powerful technique and perform high-level analysis, structural uniformity of active sites is highly desirable.

*Chin. J. Catal.*, 2017, 38: 1489–1497 doi: 10.1016/S1872-2067(17)62799-2

### Increasing the range of non-noble-metal single-atom catalysts

Ting Deng, Weitao Zheng \*, Wei Zhang \*  
Jilin University, China; CIC Energigune, Parque Tecnológico de Álava, Spain; Ikerbasque, Basque Foundation for Science, Spain



The catalytic performances of non-noble metals are inferior to those of noble metals. The advent of single-atom catalysts (SACs) has shifted the balance. Experimental and theoretical studies have shown that non-noble-metal SACs have a promising future in various key reactions.

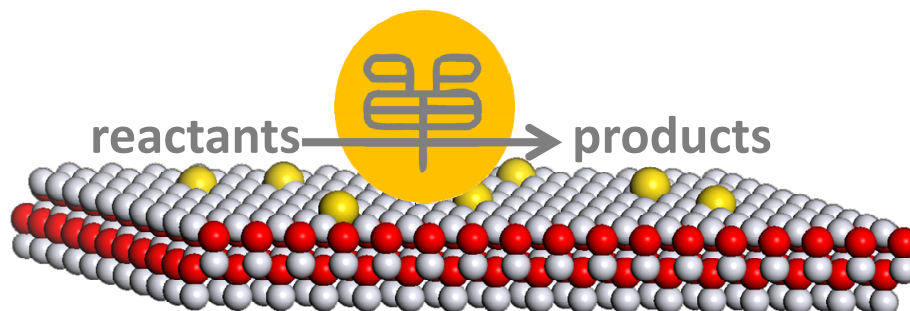
## Minireviews

*Chin. J. Catal.*, 2017, 38: 1498–1507 doi: 10.1016/S1872-2067(17)62872-9

### Highlights of the major progress in single-atom catalysis in 2015 and 2016

Bing Han, Rui Lang, Botao Qiao\*, Aiqin Wang, Tao Zhang

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



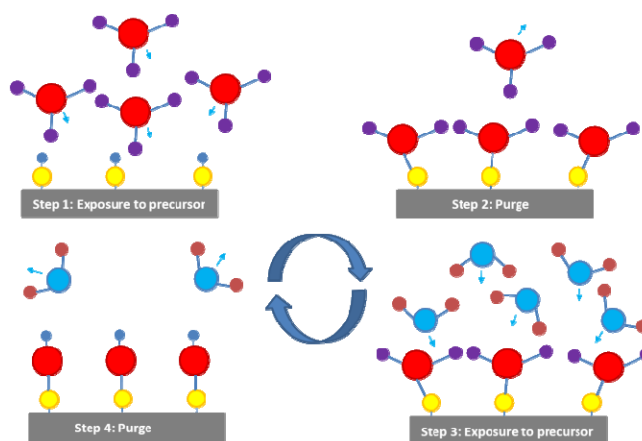
The latest developments in single-atom catalysis are highlighted, including new approaches in single-atom catalyst (SAC) synthesis, stable gold SACs, highly selective platinum and palladium SACs, and non-noble metal SACs in electrochemistry.

*Chin. J. Catal.*, 2017, 38: 1508–1514 doi: 10.1016/S1872-2067(17)62903-6

### Single atom catalyst by atomic layer deposition technique

Niancai Cheng, Xueliang (Andy) Sun\*

*University of Western Ontario, Canada; Fuzhou University, China*



This review summarizes recent development of single atom catalyst synthesized by atomic layer deposition and explores future research directions and trends.

## Reviews

*Chin. J. Catal.*, 2017, 38: 1515–1527 doi: 10.1016/S1872-2067(17)62782-7

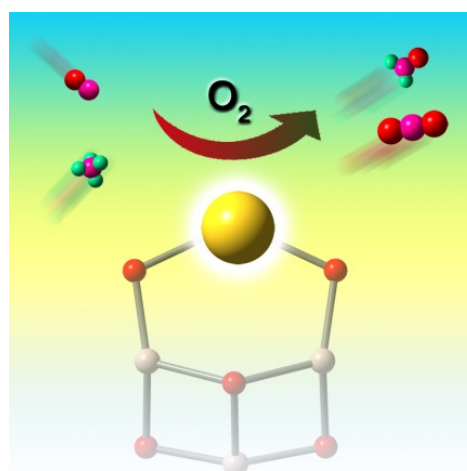
### Metal-mediated catalysis in the gas phase: A review

Xiao-Na Li, Xiu-Ping Zou, Sheng-Gui He\*

*Institute of Chemistry, Chinese Academy of Sciences;*

*South China University of Technology*

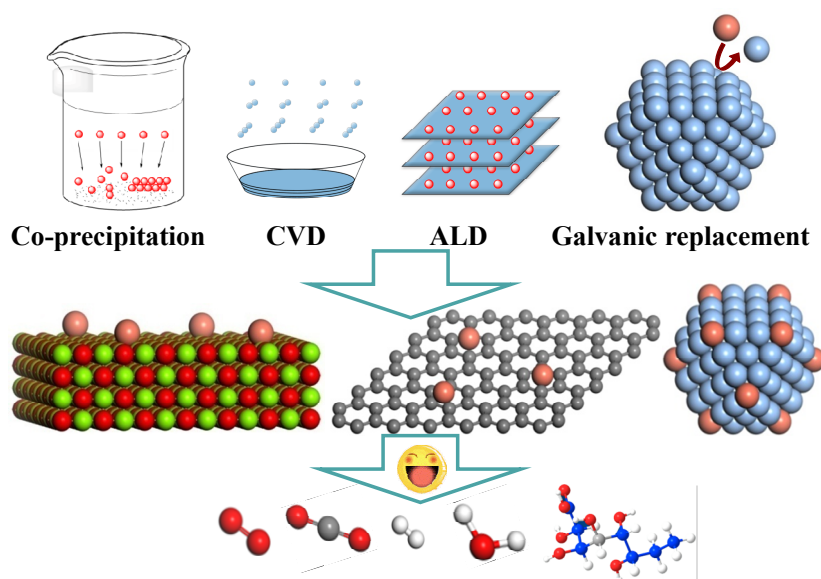
In this review, the experimentally identified gas-phase catalytic cycles mediated by atomic metal ions, bare metal clusters, metal oxide clusters, and metal complexes are summarized with an emphasis on the reactivity of cluster confined single-atom catalysts.



*Chin. J. Catal.*, 2017, 38: 1528–1539 doi: 10.1016/S1872-2067(17)62770-0

### Preparation, characterization and catalytic performance of single-atom catalysts

Liqiong Wang, Liang Huang\*, Feng Liang, Simin Liu, Yuhua Wang, Haijun Zhang\*  
Wuhan University of Science and Technology



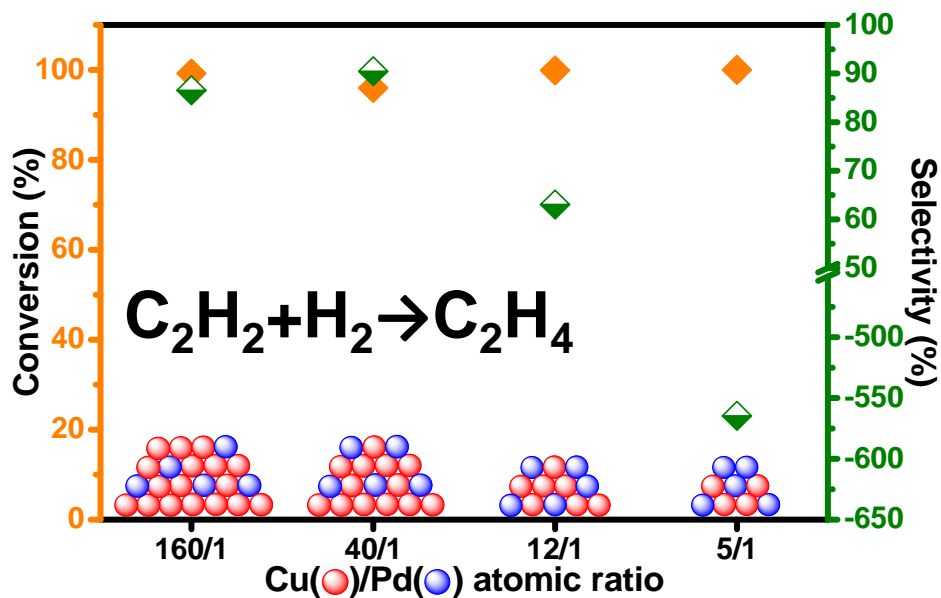
Single-atom catalysts (SACs) have become a desirable research topic. The preparation, characterization and catalytic performance of three kinds of SACs with single atoms anchored onto metal oxides, two-dimensional materials and metal nanoclusters are summarized.

## Articles

*Chin. J. Catal.*, 2017, 38: 1540–1548 doi: 10.1016/S1872-2067(17)62847-X

### Isolation of Pd atoms by Cu for semi-hydrogenation of acetylene: Effects of Cu loading

Guangxian Pei, Xiaoyan Liu\*, Mengqian Chai, Aiqin Wang, Tao Zhang\*  
Dalian Institute of Chemical Physics, Chinese Academy of Sciences; University of Chinese Academy of Sciences

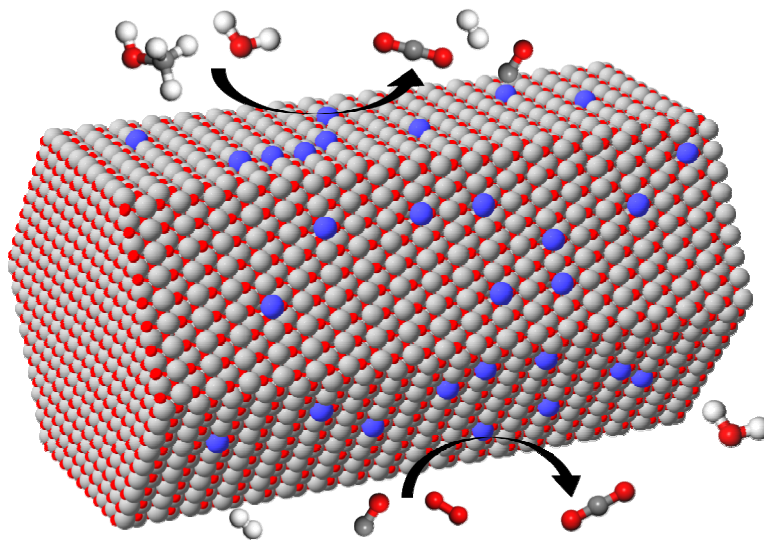


Cu-alloyed Pd single-atom catalysts were formed for Cu/Pd atomic ratios  $\geq 40/1$  and displayed excellent catalytic performance for the semi-hydrogenation of acetylene in excess ethylene.

*Chin. J. Catal.*, 2017, 38: 1549–1557 doi: 10.1016/S1872-2067(17)62899-7

### Probing the catalytic behavior of ZnO nanowire supported Pd<sub>1</sub> single-atom catalyst for selected reactions

Jia Xu, Yian Song, Honglu Wu, Jingyue Liu \*  
Arizona State University, United States; Beijing Jiaotong University, China

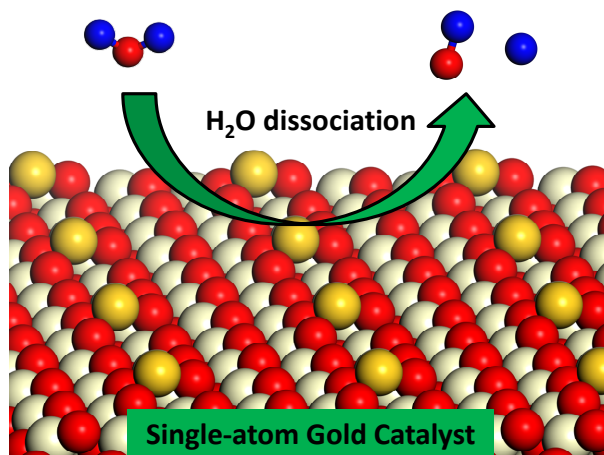


ZnO nanowire supported Pd single-atom catalysts (SACs) were synthesized and evaluated for selected catalytic reactions and the Pd<sub>1</sub>/ZnO SAC demonstrated excellent activity and selectivity for steam reforming of methanol to produce hydrogen.

*Chin. J. Catal.*, 2017, 38: 1558–1565 doi: 10.1016/S1872-2067(17)62829-8

### Investigation of water adsorption and dissociation on Au<sub>1</sub>/CeO<sub>2</sub> single-atom catalysts using density functional theory

Yan Tang, Yang-Gang Wang \*, Jin-Xia Liang, Jun Li \*  
Tsinghua University; Guizhou Normal College



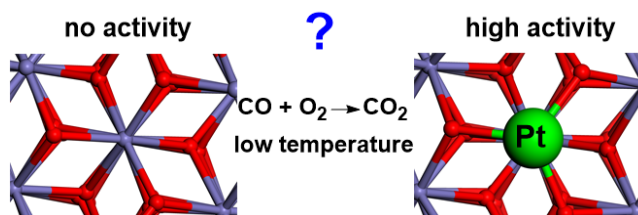
Positively charged single-atom Au on ceria support is a potential catalyst for water dissociation. It can not only provide the activation site for water adsorption but also facilitate water dissociation by weakening the intramolecular O–H bond.

*Chin. J. Catal.*, 2017, 38: 1566–1573 doi: 10.1016/S1872-2067(17)62879-1

### Catalytic activities of single-atom catalysts for CO oxidation: Pt<sub>1</sub>/FeO<sub>x</sub> vs. Fe<sub>1</sub>/FeO<sub>x</sub>

Jinxia Liang, Xiaofeng Yang \*, Congqiao Xu, Tao Zhang, Jun Li \*  
Guizhou Education University; Tsinghua University;  
Dalian Institute of Chemical Physics, Chinese Academy of Sciences

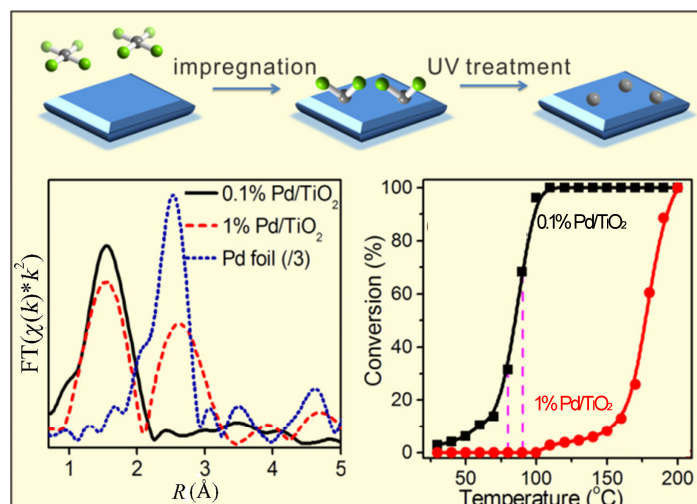
Pt<sub>1</sub>/FeO<sub>x</sub> has higher catalytic activity for CO oxidation than that of the FeO<sub>x</sub> substrate alone because the regeneration of oxygen vacancies features a high activation barrier for desorption of a second CO<sub>2</sub> molecule at the surface of Fe<sub>1</sub>/FeO<sub>x</sub> (i.e., the FeO<sub>x</sub> substrate).



*Chin. J. Catal.*, 2017, 38: 1574–1580 doi: 10.1016/S1872-2067(17)62784-0

### Photochemical route for preparing atomically dispersed Pd<sub>1</sub>/TiO<sub>2</sub> catalysts on (001)-exposed anatase nanocrystals and P25

Pengxin Liu, Jie Chen, Nanfeng Zheng\*  
Xiamen University



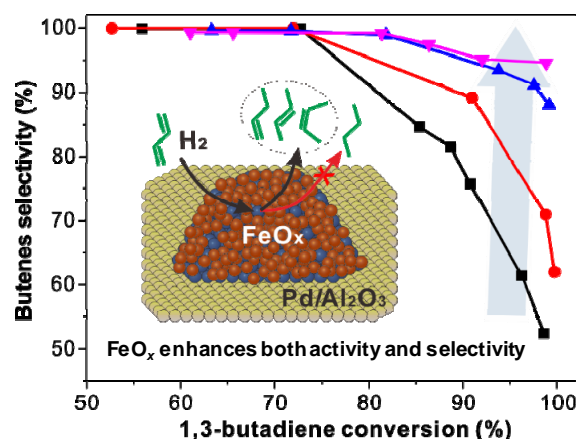
Pd<sub>1</sub>/TiO<sub>2</sub> catalysts prepared via a photochemical route showed excellent catalytic activities and stabilities in both styrene hydrogenation and CO oxidation.

*Chin. J. Catal.*, 2017, 38: 1581–1587 doi: 10.1016/S1872-2067(17)62768-2

### Coating Pd/Al<sub>2</sub>O<sub>3</sub> catalysts with FeO<sub>x</sub> enhances both activity and selectivity in 1,3-butadiene hydrogenation

Hong Yi, Yujia Xia, Huan Yan, Junling Lu\*  
University of Science and Technology of China

Deposition of FeO<sub>x</sub> onto Pd/Al<sub>2</sub>O<sub>3</sub> catalyst can remarkably improve both hydrogenation activity and butenes selectivity through the electronic effect and geometric effect, respectively.

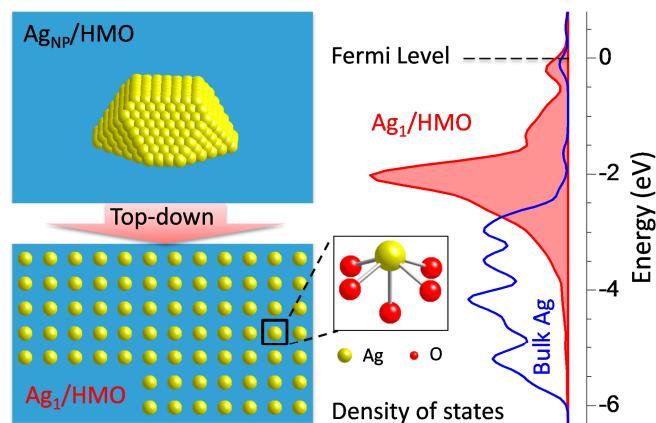


*Chin. J. Catal.*, 2017, 38: 1588–1596 doi: 10.1016/S1872-2067(17)62778-5

### Top-down synthesis strategies: Maximum noble-metal atom efficiency in catalytic materials

Yaxin Chen, Zhiwei Huang, Xiao Gu, Zhen Ma, Jianmin Chen,  
Xingfu Tang\*  
Fudan University;  
Congqing University;  
Nanjing University of Information Science & Technology

The top-down strategy is successfully used to synthesize atomically dispersed metal catalysts from supported Ag nanoparticles by a thermal diffusion process. The driving force is attributed to the electronic perturbation of the Ag frontier orbitals.

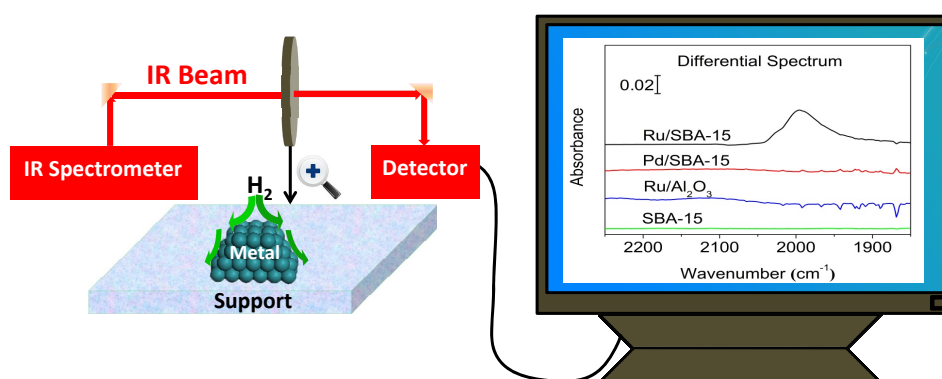




*Chin. J. Catal.*, 2017, 38: 1597–1602 doi: 10.1016/S1872-2067(16)62571-8

### Identification of active sites for hydrogenation over Ru/SBA-15 using *in situ* Fourier-transform infrared spectroscopy

Hangjia Shen, Xianyuan Wu, Dahao Jiang, Xiaonian Li, Jun Ni\*  
Zhejiang University of Technology

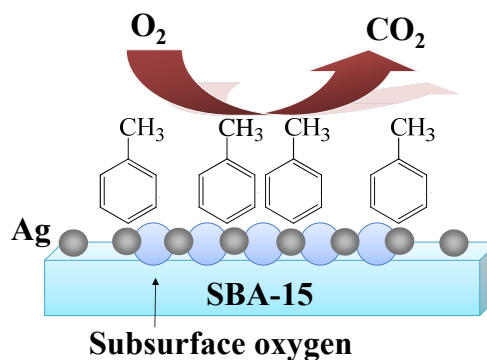


The active sites for hydrogenation over Ru/SBA-15 catalysts were identified using *in situ* FTIR spectroscopy. The formation of these active sites is probably an intermediate step in hydrogen spillover.

*Chin. J. Catal.*, 2017, 38: 1603–1612 doi: 10.1016/S1872-2067(17)62842-0

### Effect of pretreatment conditions on catalytic activity of Ag/SBA-15 catalyst for toluene oxidation

Yuan Qin, Zhenping Qu\*, Cui Dong, Na Huang  
Dalian University of Technology

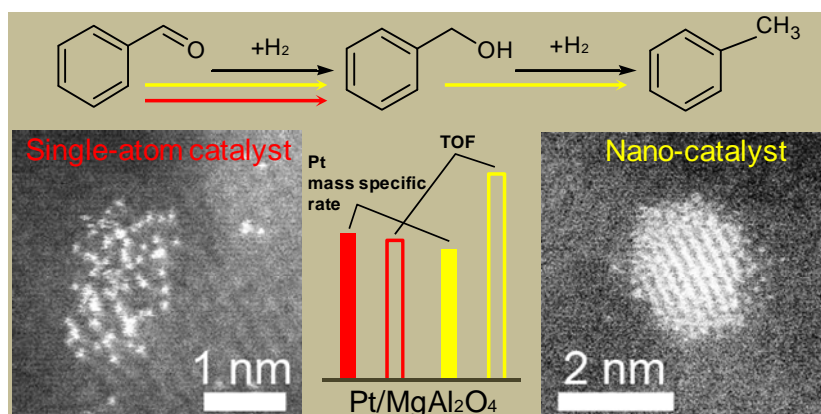


Redispersed, small Ag particles on the O500-H300 sample show high activation ability for O<sub>2</sub> and great affinity with toluene because of the formation of subsurface oxygen, leading to high catalytic activity for toluene oxidation.

*Chin. J. Catal.*, 2017, 38: 1613–1620 doi: 10.1016/S1872-2067(17)62815-8

### Effect of the degree of dispersion of Pt over MgAl<sub>2</sub>O<sub>4</sub> on the catalytic hydrogenation of benzaldehyde

Feng Yan, Caixian Zhao, Lanhua Yi\*, Jingcai Zhang, Binghui Ge, Tao Zhang, Weizhen Li\*  
Xiangtan University; Dalian Institute of Chemical Physics, Chinese Academy of Science; Institute of Physics, Chinese Academy of Science

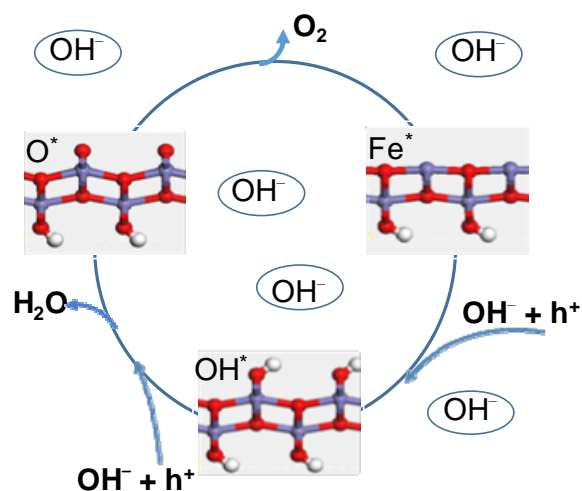


MgAl<sub>2</sub>O<sub>4</sub>-supported Pt single-atom catalysts are highly active in the selective hydrogenation of benzaldehyde to benzyl alcohol. Pt nanocatalysts are more active but less selective, presumably because of the formation of Pt terraces.

*Chin. J. Catal.*, 2017, 38: 1621–1628 doi: 10.1016/S1872-2067(17)62760-8

**Mechanistic understanding on oxygen evolution reaction on  $\gamma$ -FeOOH (010) under alkaline condition based on DFT computational study**

Miru Tang, Qingfeng Ge\*  
Southern Illinois University, USA

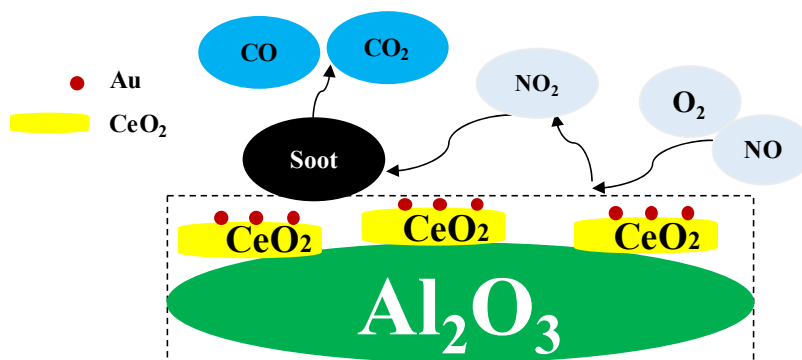


Oxygen evolution mechanism on FeOOH (010) catalyst under the alkaline condition. The circled  $OH^-$  represent hydroxide ions in solution. Blue sphere is Fe, red O and white H.

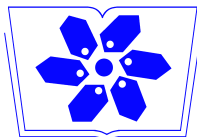
*Chin. J. Catal.*, 2017, 38: 1629–1641 doi: 10.1016/S1872-2067(17)62798-0

**Three-dimensionally ordered macroporous  $CeO_2/Al_2O_3$ -supported Au nanoparticle catalysts: Effects of  $CeO_2$  nanolayers on catalytic activity in soot oxidation**

Baofang Jin, Yuechang Wei\*, Zhen Zhao\*, Jian Liu, Yazhao Li, Renjie Li, Aijun Duan, Guiyuan Jiang  
China University of Petroleum (Beijing); Shenyang Normal University



A mixed oxide catalyst containing Au,  $CeO_2$ , and  $Al_2O_3$  combines the benefits of high activity, good redox properties, and high surface area, and provides a highly effective catalyst for soot oxidation.



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## 单原子催化国际研讨会专刊

客座主编: 张涛, 刘景月, 李隽

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