

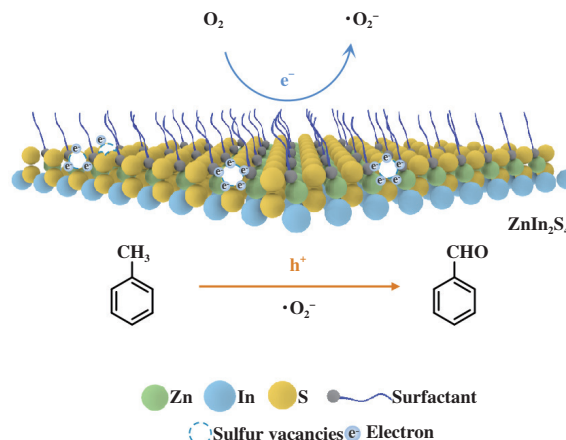
### Photocatalytic Selective Oxidation of Toluene over Surfactant-Modified ZnIn<sub>2</sub>S<sub>4</sub>

DI Lu, ZHAO Sheng-nan, LI Xin-gang

J. Mol. Catal. (China) **2022**, 36(5): 413~424

We report visible-light-driven photocatalytic selective oxidation of toluene over surfactant-modified ZnIn<sub>2</sub>S<sub>4</sub> semiconductors. All samples were characterized by TEM, XRD, UV-vis, ESR, and photoelectrochemical performance test. The modification with surfactant assists the formation of sulfur vacancies on ZnIn<sub>2</sub>S<sub>4</sub>, and enhances the separation efficiency of charge carrier, thereby significantly increasing the photocatalytic

activity.



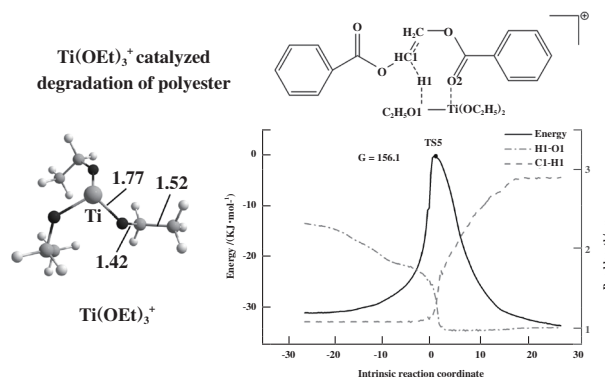
### DFT Study on the Mechanism of Thermal Degradation of Polyester

ZHANG Jia-long, GUAN Zhen-yu, ZHU You-cai, LIU Zhen

J. Mol. Catal. (China) **2022**, 36(5): 425~432

The mechanism of thermal degradation of polyester by Ti-based catalyst was investigated by density functional theory (DFT) calculations. The Lewis acid catalyzed thermal degradation mechanism (M1 mechanism) and the alkoxy ligand assisted thermal degradation mechanism (M2 mechanism) were investigated for the depolymerization of ethylene dibenzoate (EDB) catalyzed by Ti(OEt)<sub>4</sub> and the cationic Ti(OEt)<sub>3</sub><sup>+</sup>, respectively. The calculations showed that the activation energy barriers for the Lewis acid catalyzed thermal degradation by both catalysts is similar to the barrier in the absence of the catalyst.

The cationic Ti(OEt)<sub>3</sub><sup>+</sup> significantly reduced the activation barrier for thermal degradation of EDB (M2 mechanism), which is believed to be the active center for the depolymerization of EDB. The principal interacting orbital (PIO) analysis revealed more orbital interactions between the cationic catalyst and the EDB polyester.



### Study on the Electronic Structure Modulation and Photocatalytic Performance of Bismuth Oxychloride Photocatalysts

ZHANG Hao-yu, GUO Ji-wei, GONG Jian-ren, XIN xin,  
LI Hua-wei, YANG Jia-min, HUANG Shu-shu

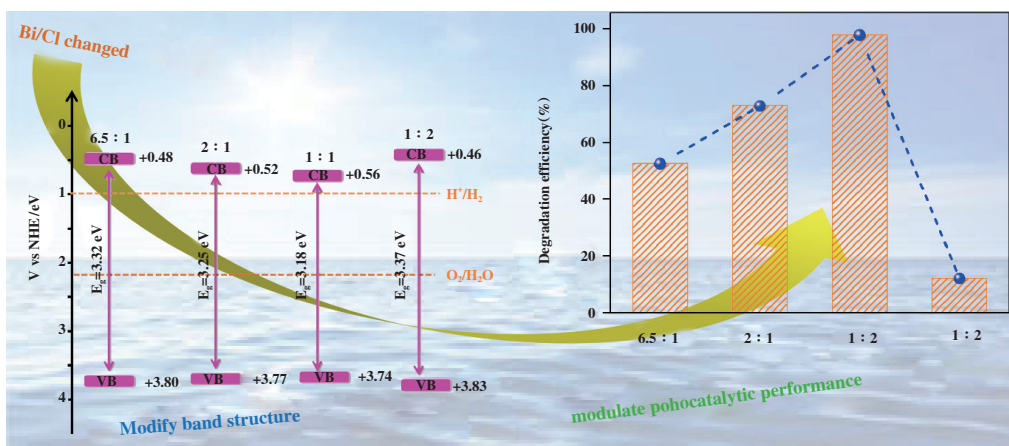
J. Mol. Catal. (China) **2022**, 36(5): 433~445

A series of BiOCl photocatalysts were prepared aiming to study the effect of Bi/Cl molar ratio on the morphologies, micro-electronic structure and photocatalytic performance. Oxygen vacancies (OVs) were successfully induced into BiOCl semiconductor by changing Bi/Cl, being confirmed by electron paramagnetic resonance (EPR) measurement, which were

beneficial to enhancing visible light absorption ability and the separation efficiency of photogenerated charge carriers. The results of X-ray photoelectron spectroscopy (XPS) demonstrated that BiOCl sample with Bi : Cl=1 : 1 had a higher content of OVs, which was further verified by EPR analysis. Meanwhile, steady state fluorescence spectroscopy (PL) and transient fluorescence spectroscopy (TRPL) analysis declared that Bi : Cl=1 : 1 sample owned a lower PL intensity and a smaller average lifetime of photoelectron, indicating a higher separation efficiency of photogenerated electron-hole pairs. Hence, Bi : Cl=1 : 1 sample owned the optimal photocatalytic RhB degradation activity with a removal efficiency of 98.0%. Furthermore, the TOC of RhB was decreased to 55.81% after the adsorption and photocatalytic degradation process, indicating photocatalytic

degradation could destroy the organic groups of RhB and partially convert them into  $\text{CO}_2$  and  $\text{H}_2\text{O}$ . A decreased reactive rate of photocatalytic degradation RhB after three reaction cycles indicated that the photocatalytic stability of BiOCl needed to be

further improved. A series of controlled experiments by adding different active species scavengers showed that photogenerated electrons, holes and  $\cdot\text{O}_2^-$  active species contributed together for photocatalytic degradation RhB.



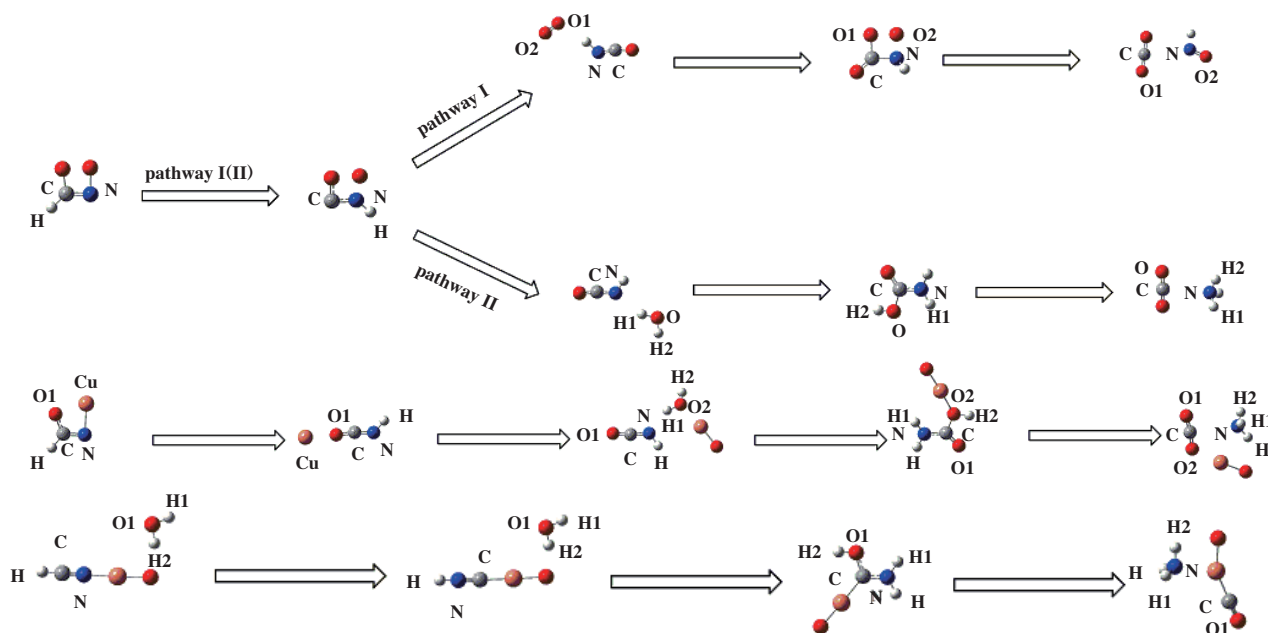
### Theoretical Study on the Reaction Mechanism of HCN Elimination

PENG Guo-jian, YANG Meng, WANG Guo-wei, LIU Yong-jun, YANG Chun-xiao, ZHANG Yan-kun, XIA Fu-ting

J. Mol. Catal. (China) **2022**, 36(5): 446~455

In order to reveal the mechanism of HCN elimination reaction, the direct elimination of HCN and the catalytic elimination of HCN on CuO were studied from the perspectives of HCN

oxidation and hydrolysis by density functional theory. In pathway I, HCN reacts with one  $\text{O}_2$  molecule to form HNCO, and the products of HNCO oxidation are  $\text{CO}_2$ , NO and H atom. In pathway II, HCN reacts with one  $\text{O}_2$  molecule to form HNCO, and the products of HNCO hydrolysis are  $\text{CO}_2$  and  $\text{NH}_3$ . In pathway III, HCN reacts with CuO to form HNCO, and the products of HNCO hydrolysis on CuO are  $\text{CO}_2$  and  $\text{NH}_3$ . In pathway IV, the products of HCN hydrolysis on CuO are CO and  $\text{NH}_3$ . It is shown that the optimal way to eliminate HCN was to decompose into  $\text{CO}_2$  and  $\text{NH}_3$  on CuO.

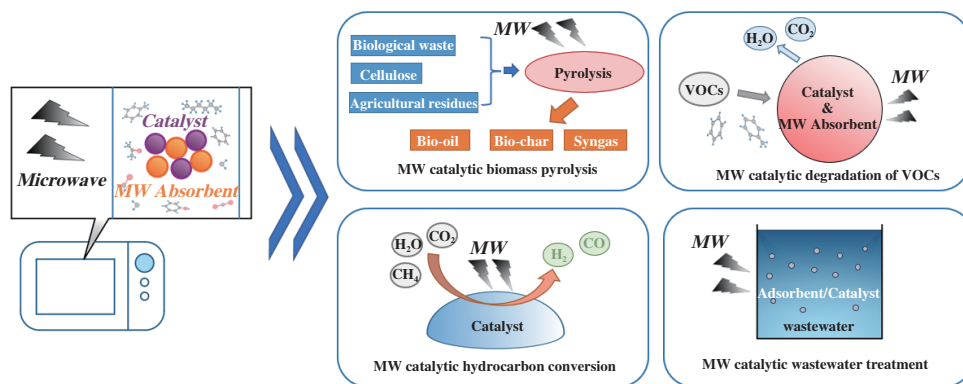


## Microwave Catalysis for Energy and Environment: A Review

FANG Dong-xu, LIU Zhi-xi, JIANG Zhi

J. Mol. Catal. (China) **2022**, 36(5): 456~466

Microwave (MW) energy can be absorbed by materials via various loss mechanisms. The coexistence of multiple loss modes can significantly improve the heating property of materials under MW, which is crucial for optimizing the MW catalytic process.



MW is therefore considered as a green and efficient form of energy and widely used in catalytic processes in the fields of energy and environment. In this article, recent progresses of MW catalysis were reviewed, especially for different application scenario, such as volatile organic compounds (VOCs) removal, biomass pyrolysis, the reforming of methane and carbon oxides and wastewater treatment. Besides, recent studies on the mechanism of MW catalysis including “thermal/non-thermal effect” and “hot spot” were also discussed in this article.

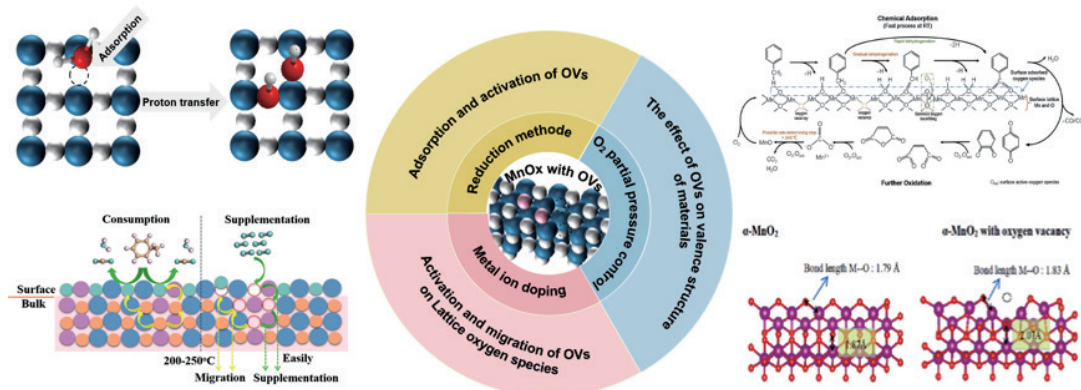
## Research Progress on the Construction of Oxygen Vacancies in Manganese Oxides and the Mechanism of Their Catalytic Oxidation of Benzene Series

LIAO Wei, LU Ji-chang, ZHANG Ying, LIU Jiang-ping, LUO Yong-ming, ZHU Wen-jie

J. Mol. Catal. (China) **2022**, 36(5): 467~479

Manganese oxides has a very wide range of applications in the field of catalytic oxidation of benzene series. At present, most studies mainly adjust their physicochemical properties from the crystal form, morphology, and crystal plane of manganese oxides, thereby improving their catalytic performance. But no matter from which point of view, there is an inseparable relationship with

oxygen vacancies (OVs) to a large extent. Meanwhile, transition metal oxides usually follow the MVK mechanism, in which OVs play an important role in the activation of oxygen and the replenishment of lattice oxygen. With the deepening of related research, more evidences show that oxygen vacancies can promote the catalytic oxidation of benzene series from various aspects. This paper reviews the method of establishing common OVs, including reduction method (gas-phase reduction, liquid-phase reduction and solid-phase reduction), heterometal ion doping, oxygen partial pressure adjustment, and summarizes the effects of OVs in manganese oxides on the adsorption and activation of oxygen, water molecules and benzene series, on the activation and migration of lattice oxygen, and on the valence structure of manganese oxides.



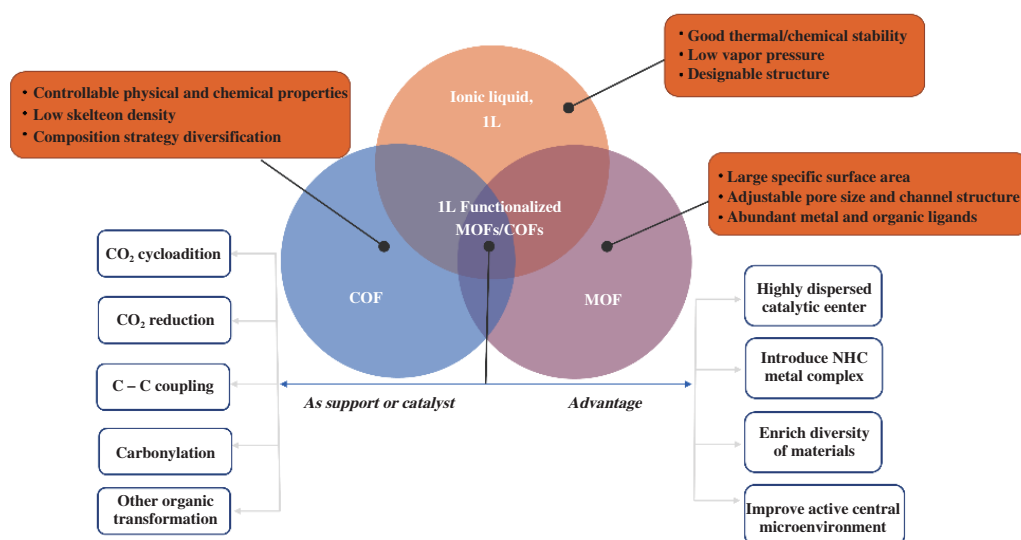
### Application of Ionic Liquid Functionalized MOFs/COFs in Catalytic Reactions

LAN Yong-cheng, LU Yan-mei, YUN Dong, XIA Chun-gu, LIU Jian-hua

J. Mol. Catal. (China) **2022**, 36(5): 480~498

Ionic liquids (ILs) functionalized metal organic frameworks (MOFs) and covalent organic frameworks (COFs) composites are promising catalytic materials. Abundant pore structure and ultra-high specific surface area of MOFs and COFs provide a platform

for uniformly dispersed catalytic active centers, and promote the mass transfer process of reaction substrates and products, thus achieving efficient catalytic reaction. The introduction of ionic liquid effectively improves the microenvironment of the frame material, in addition, it can also be converted to NHC under appropriate conditions. Therefore, the application of MOFs or COFs functionalized catalytic systems for ionic liquids in CO<sub>2</sub> cycloaddition, application of CO<sub>2</sub> reduction functionalization, C—C coupling, carbonylation reactions and other organic conversion reactions in recent years are briefly reviewed.



### The State of the Art Review on the Photo-thermal Reactor of CO<sub>2</sub> Reduction

TANG Wen-bin, ZHANG Zhi-xiang, CHI Jia-sheng, CHEN Ming-xia, JIANG Zhi, SHANGGUAN Wen-feng

J. Mol. Catal. (China) **2022**, 36(5): 499~512

Photothermal catalytic reduction is a very promising technology route for CO<sub>2</sub> resource utilization. Light can excite the reactants and effectively reduce the temperature and activation energy required for the reaction, while the thermal effect can increase the rate of diffusion adsorption, electron transfer and chemical reactions of the reactants, provide the energy required to cross the activation energy barrier, promote the catalytic reduction of CO<sub>2</sub> and make defects such as oxygen vacancies into important active sites. Synergizing light and heat to promote each other can compensate for the defects of a single reaction. Designing efficient new catalyst materials and developing reactors compatible with catalytic materials to maximize the catalyst performance are

the keys to photothermal catalytic amplification reactions. The development of catalysts and the design of reactors are still in their infancy and require the design of reactors in terms of reactor structure, reactor operation, control and precise monitoring of heating, and precise control of light intensity. Combining microfluidic channels, photonic elements, and increasingly high-precision thermal controllers and detectors, the performance of catalysts is fully utilized. With the continuous development of high-efficiency catalysts and reactors, it is expected to contribute to the achievement of the strategic goal of carbon neutrality.

