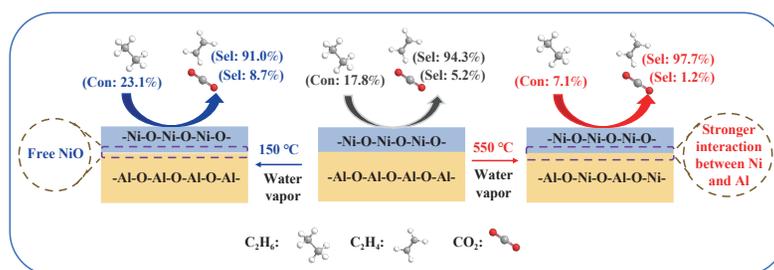


### The Influence of Water Vapor Treating Temperature on Ni-Ga/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> for Oxidative Dehydrogenation of Ethane to Ethylene

LI Qinghui, ZHAO Huahua, YANG Jian, ZHAO Jun,  
YAN Liang, SONG Huanling, CHOU Lingjun

J. Mol. Catal. (China) **2025**, 39(1): 001–013.

The Ni-Ga/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst was prepared using the impregnation method and then treated with water vapor at different temperature (150–550 °C). Low-temperature water vapor treatment ( $\leq 350$  °C) was more conducive to the generation of free NiO, benefiting the improvement of ethane conversion and CO<sub>2</sub> production. Further increasing the temperature of water vapor treatment ( $\geq 450$  °C) strengthened the interaction between metal and support, which could lead to the formation of NiAl<sub>2</sub>O<sub>4</sub>, as well as in favor of the improvement of ethylene selectivity.



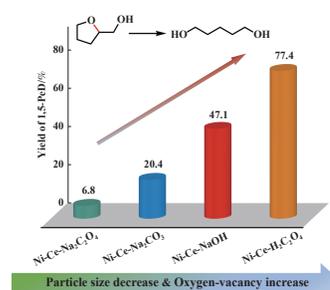
### Effect of Precipitators on Selective Hydrogenation Ring-opening of Tetrahydrofurfuryl Alcohol over Ni-Ce Catalysts

LIU Qi, LI Fuwei, SUN Peng, GAO Guang, XI Yongjie,  
ZHAO Zelun, HUANG Zhiwei

J. Mol. Catal. (China) **2025**, 39(1): 014–022.

A series of Ni-Ce catalysts were prepared by coprecipitation method under different precipitators (Ni-Ce-p, p=Na<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, Na<sub>2</sub>CO<sub>3</sub>, NaOH, H<sub>2</sub>C<sub>2</sub>O<sub>4</sub>), which the structures were determined by SEM, XRD, Raman, H<sub>2</sub>-TPR and quasi *in-situ* XPS characterization. The results showed that the Ni-Ce-H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> catalyst had higher catalytic activity for tetrahydrofurfuryl

alcohol (THFA) hydrogenation to 1,5-pentanediol (1,5-PeD) because of the smaller particle size and high concentration of oxygen-vacancies, which the yield of 1,5-PeD was about 11.4 times higher than that of the Ni-Ce-Na<sub>2</sub>C<sub>2</sub>O<sub>4</sub> catalyst. This work provides a promising method for regulating catalytic activity by changing the structure of catalysts with different precipitators.



### Investigating the Effect of MoS<sub>2</sub> Hydrothermal Synthesis Factors on CO<sub>2</sub> Hydrogenation to Methanol

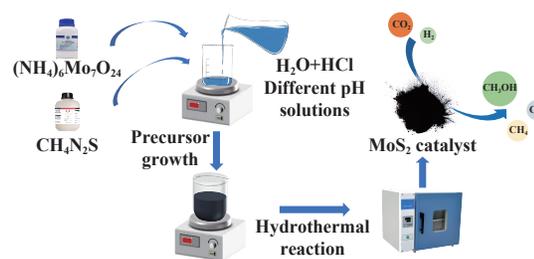
WEN Changhong, DING Mingshan, LIU Na, HUANG Xueli,  
HUANG He

J. Mol. Catal. (China) **2025**, 39(1): 023–033.

The process of low-temperature hydrogenation of CO<sub>2</sub> to methanol is of significant importance in the recycling of greenhouse gases into valuable products. The structure of MoS<sub>2</sub>, an efficient catalyst for the catalytic hydrogenation of

CO<sub>2</sub> to methanol, has a considerable influence on the catalytic performance. The preparation of structurally controllable MoS<sub>2</sub> nanosheets was conducted *via* the hydrothermal method. The impact of varying the Mo/S molar ratio, the pH of the precursor solution and the duration of the precursor growth phase on the structure and properties of the MoS<sub>2</sub> nanosheets was examined. The MoS<sub>2</sub> nanosheets were characterized using XRD, SEM, BET analysis and XPS, and the catalytic activity in the CO<sub>2</sub> hydrogenation to methanol reaction was investigated. The results showed that the prepared MoS<sub>2</sub> catalysts with clear layered structure and high crystallinity at Mo/S molar ratio of 1/4, precursor solution pH of 1.4 and precursor growth time of

12 h exhibited the best catalytic activity for CO<sub>2</sub> hydrogenation to methanol, with a CO<sub>2</sub> conversion of 4.35% and a methanol selectivity of 59.93%. This work provides an experimental basis and theoretical foundation for the design and research of related catalyst materials.



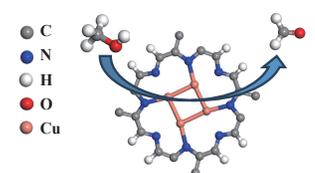
### DFT Study on Adsorption and Cracking Mechanism of Methanol on the Cu<sub>4</sub>-C<sub>5</sub>N<sub>2</sub>H<sub>2</sub> Surface

WANG Wannan, REN Ruipeng, LÜ Yongkang

J. Mol. Catal. (China) **2025**, 39(1): 034–040.

Formaldehyde is extensively utilized in the production of cosmetics, food products, health items, and industrial chemicals. The non-oxidative direct dehydrogenation of methanol to formaldehyde presents a promising approach. Using Cu<sub>4</sub> cluster embedded in carbon nitride (Cu<sub>4</sub>-C<sub>5</sub>N<sub>2</sub>H<sub>2</sub>) as catalyst model, the mechanism of methanol adsorption and cracking on the catalyst surface was explored based on DFT-D3. It is found that Cu<sub>4</sub>-C<sub>5</sub>N<sub>2</sub>H<sub>2</sub> exhibits excellent stability and

high formaldehyde selectivity. The optimal pathway of methanol cracking is CH<sub>3</sub>OH→CH<sub>3</sub>O→CH<sub>2</sub>O, and the rate-limiting step is CH<sub>3</sub>O→CH<sub>2</sub>O. The energy barrier and rate constant corresponding to this elementary reaction are 0.89 eV and 1.70×10<sup>6</sup> s<sup>-1</sup>, respectively. The charge analysis results showed that the electron transfer between the catalyst and methanol activated the methanol, which further reacted to form formaldehyde.



CH<sub>3</sub>OH to CH<sub>2</sub>O on the Cu<sub>4</sub>-C<sub>5</sub>N<sub>2</sub>H<sub>2</sub> surface

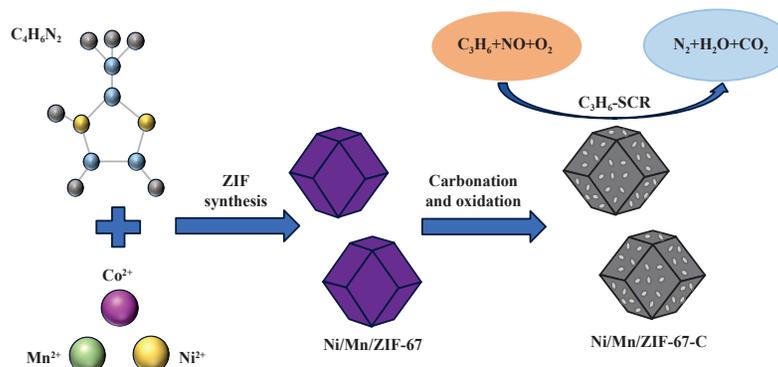
### Research on the C<sub>3</sub>H<sub>6</sub>-SCR DeNO<sub>x</sub> Characteristics of MOF-Derived Ni/Mn/CoO<sub>x</sub>-C Catalyst

LI Juxing, ZHANG Jinwei, NING Shuying, HU Mingtao, SU Yaxin

J. Mol. Catal. (China) **2025**, 39(1): 041–052.

As environmental regulations become increasingly stringent, the control of nitrogen oxides (NO<sub>x</sub>) emissions has emerged as an important research direction in the industrial and transportation sectors. The metal-organic framework (MOF) material ZIF-67, with its superior tunable structure and rich

porous characteristics, has become an ideal candidate for catalyst development. In this study, we successfully synthesized Mn and Ni-modified ZIF-67 using a co-precipitation method, followed by carbonization and oxidation-derived steps to produce the Ni/Mn/CoO<sub>x</sub>-C catalyst. Performance testing for C<sub>3</sub>H<sub>6</sub> selective catalytic reduction (SCR) was conducted under rich oxygen conditions (O<sub>2</sub> volume fraction 5%). The results indicated that the synthesized catalyst achieved a NO conversion rate of 93.2% at 225 °C, while maintaining an N<sub>2</sub> selectivity of over 86%, demonstrating that bimetallic doping significantly enhances the catalyst activity and selectivity. Characterization analyses revealed that the synergistic doping of Ni and Mn improved the redox properties of the catalyst, effectively enhancing its overall activity.



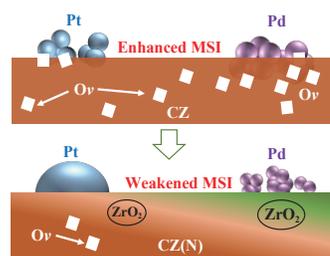
### Influence of Support Pretreatment on Pt and Pd-based TWCs Performance

ZHANG Jun, CHEN Liuling, SU Min, JIAO Yi, WANG Jianli, HU Zhibiao, ZHANG Xinbo, JI Cunmin, ZHENG Heng

J. Mol. Catal. (China) **2025**, 39(1): 053–064.

Metal-support interaction (MSI) can change metal chemical state, which is closely related to three-way catalyst (TWCs) performance. The CeO<sub>2</sub>-ZrO<sub>2</sub>(CZ) support was pretreated by both heat treatment and NaBH<sub>4</sub> etching to modulate the MSI of Pt-CZ and Pd-CZ. The heat treatment significantly enhance the high-temperature stability of Pt/CZ, whereas the activity of Pd/CZ was observed to decrease. NaBH<sub>4</sub> etching made the Pt/CZ catalyst appeared to be phased, the MSI was weakened. And the reduced interaction caused the

sintering of Pt particles. For Pd/CZ, on the contrary, the weaker interaction facilitated to the conversion of Pd species into active species, thereby promoting catalytic activity. In addition, the change of oxygen vacancy content induced by support pretreatment was positively correlated with the MSI intensity, and the oxygen vacancy content in the catalyst was higher following heat treatment compared to NaBH<sub>4</sub> etching of CZ support. By elucidating the relationship between MSI and the performance of TWCs, this work provides a new idea for a deeper understanding of support optimization to regulate MSI.



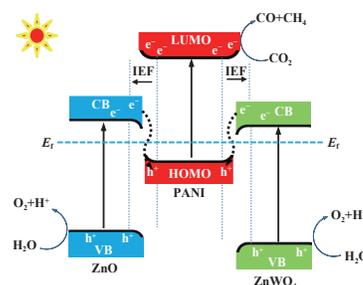
### PANI Induced ZnO@ZnWO<sub>4</sub> to Construct Double S-scheme Heterojunction for Photocatalytic CO<sub>2</sub> Reduction

LI Yuejun, CAO Tieping, SUN Dawei

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With the continuous development of industrialization, CO<sub>2</sub> produced by the excessive use of fossil fuels has led to problems such as the greenhouse effect, which has attracted great attention from the international community and a series of countermeasures have been formulated. Therefore, the research and development of technology for the reduction and recovery of CO<sub>2</sub> from the atmosphere is urgent and important. Zn-based semiconductor materials, such as ZnO and ZnWO<sub>4</sub>, are widely studied in photocatalysis. However, due to the problems of electron-hole pair fast recombination and high conduction potential, they do not have photocatalytic CO<sub>2</sub> reduction activity. In this paper, ZnO@ZnWO<sub>4</sub>/PANI composite fiber photocatalytic material was successfully prepared by using polypheniline fiber with specific morphology (PANI) as composite unit, zinc nitrate as zinc source, sodium hydroxide and ammonia as mineralizer. XRD, SEM, TEM, UV-Vis DRS

and photoluminescence spectroscopy were used to characterize the phase composition, microstructure and photoelectric properties of the composite fiber materials. The formation of double S-scheme heterojunction over ZnO@ZnWO<sub>4</sub>/PANI determined by electron EPR and photocatalytic reaction process, which not only promotes the effective separation of photogenerated electron-hole pairs, but also reduces the reduction potential of ZnO@ZnWO<sub>4</sub>, and has the capacity to photocatalytic CO<sub>2</sub> reduction. Under simulated solar irradiation for 3 h, the formation rates of CH<sub>4</sub> and CO reached to 11.88 and 3.02 μmol·g<sup>-1</sup>·h<sup>-1</sup>, respectively. Impressively, ZnO@ZnWO<sub>4</sub>/PANI delivers remarkable anti-interference performance and reusability. This achievement signifies a significant step toward developing potent Zn-based semiconductor materials photosystems for environmental purification.



### Impact of Metal Doping on the Photocatalytic Water Splitting Performance of β-Ga<sub>2</sub>O<sub>3</sub> for Hydrogen Production

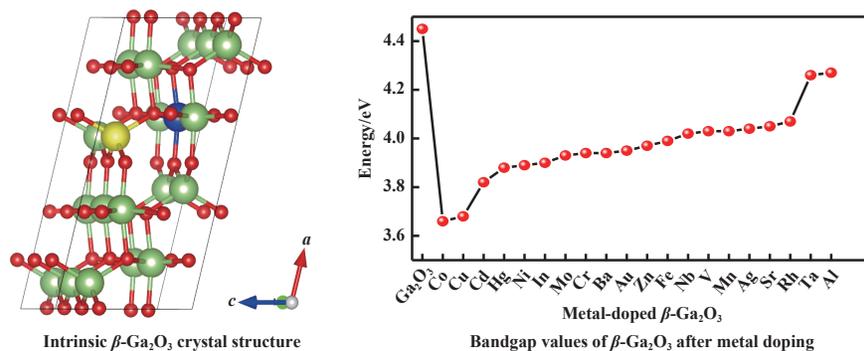
MIAO Ruixia, NIU Jiamei, YAN Jie, JIA Xiaotan

J. Mol. Catal. (China) **2025**, 39(1): 076–084.

β-Ga<sub>2</sub>O<sub>3</sub>, with its high conduction band minimum (CBM) and a low valence band maximum (VBM), possesses strong reduction and oxidation capabilities for photocatalysis. However, its wide bandgap and high carrier recombination rate limit its photocatalytic applications. Metal ion doping is considered as an effective approach to enhance the

photocatalytic performance. Using first-principles calculations, the influence of various metal ion dopants on the photocatalytic properties of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> was systematically investigated. The results show that Hg doping significantly improves the electron-

hole separation efficiency, enhances light absorption, and tunes the band edge positions, thereby boosting  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> photocatalytic performance in the visible light region.



### Research Progress in Photocatalytic Methane Conversion to High-value Products

ZHANG Runzhi, QIU Zhuo, LI Lanyan, GUO Junhao, MA Rao, GU Qianjun, YANG Zhi

J. Mol. Catal. (China) **2025**, 39(1): 085–100.

Methane is the main component of natural gas, due to its low cost, high calorific value, and vast reserves, making it a potential chemical raw material for the synthesis of high-value chemicals (oxygenates, C<sub>2+</sub> hydrocarbons, *etc.*). However, methane is recognized as the second greenhouse gas, which would result in global warming and environmental pollution. Therefore, upgrading methane to high-value products can not only reduce the content of methane in the air, but also achieve the role of protecting the environment and achieve the goal of “carbon neutrality”. At present, industrial technology mainly relies on the thermal catalysis, which demands high temperatures and pressure, leading to substantial energy usage and significant capital costs that restricts efficient methane conversion. The focus of future research is to achieve efficient conversion of methane under mild conditions. Photocatalysis offers a sustainable and environmentally friendly alternative, driven by solar energy to facilitate methane conversion at mild

temperatures, and is thus an attractive approach for producing a variety of valuable chemicals from methane. The most challenging step for activating the first C—H bond of methane in photocatalytic methane conversion is analyzed in detail. There are two ways to activate the C—H bond in methane *via* photocatalysis, i.e. photogenerated hole activation and radical activation. During the methane conversion process, the choice of photocatalytic reactor is also very important, and different catalysts need to use different reaction devices, so as to improve the yield and selectivity. It provides a research idea and reference value for the design and preparation of efficient catalysts in the future.

