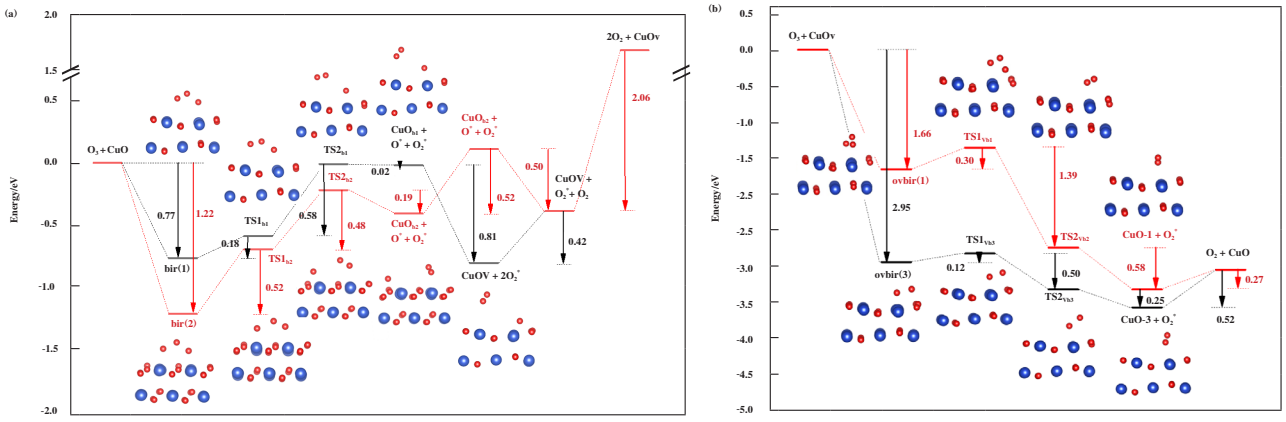
Mechanism of Ozone Decomposition and Oxygen Species Formation on Copper Oxide Surface

GONG Peng, LIU Lu, SHAO Guang-cai, WANG Guang-zhao, WANG Jun-feng

J. Mol. Catal. (China) **2022**, 36(3): 199~206

O_3 adsorption and decomposition on CuO (111) surfaces with and without oxygen vacancies were studied by density functional theory (DFT) calculations. The decomposition pathway, reaction barriers and the formation of oxygen vacancies and surface adsorbed oxygen were analyzed. The formation of oxygen vacancy improves the adsorption energy and reduces the reaction barrier. Surface active oxygen is formed during O_3 decomposition.

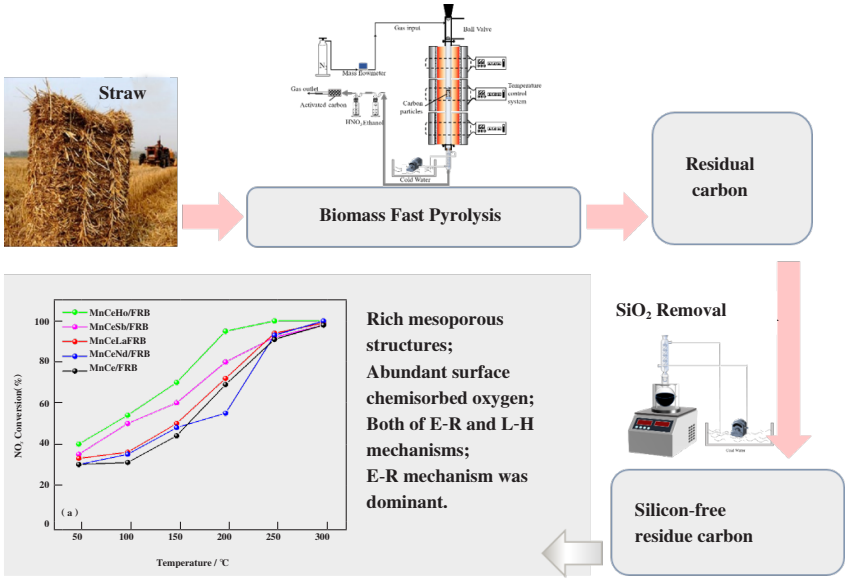


Study on the Selective Catalytic Reduction of NO by NH_3 over Silicon-free Residue Carbon Catalysts Doped with Mn-Ce-M

ZHANG Juan, WU Peng, LI Guo-bo, ZHANG Ya-ping, LI Bing-yu, YANG Hong-qiang, SHEN Kai, WANG Sheng, GONG Feng

J. Mol. Catal. (China) **2022**, 36(3): 207~220

Desiliconization not only promotes the resource utilization of silicon (more than 99% SiO_2), but also the structure of carbon materials is greatly improved (SBET up to 1923 m^2/g). Meanwhile, Ho-modified silicon-free residue carbon catalyst (MnCeHo/FRB) exhibits the best low-temperature activity (80% NO_x in the temperature range of 200~300 ℃), accompanied by the enhanced surface acidity, redox properties and abundant surface chemisorbed oxygen. Both E-R and L-H mechanisms exist over the MnCe/FRB catalysts, while E-R mechanism is dominant.

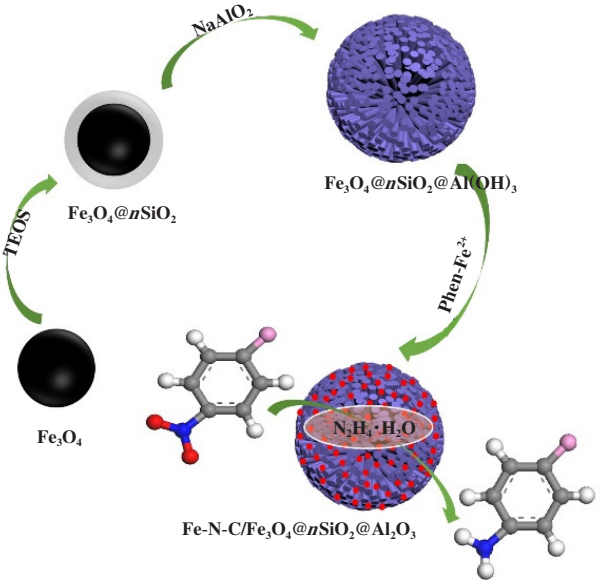


Preparation of Magnetic Mesoporous Al_2O_3 Supported Fe-N-C for the Transfer Hydrogenation of Halogenated Nitrobenzenes

ZHOU Li, LI Jun-qi, ZHANG Wei, CHEN Chao-yi, LAN Yuan-pei

J. Mol. Catal. (China) **2022**, 36(3): 221~234

Here we synthesized a magnetic mesoporous Fe-N-C/Fe_3O_4@*n*SiO_2@Al_2O_3 by calcinating 1,10-phenanthroline-Fe^{2+} (Phen-Fe^{2+}) on magnetic mesoporous Fe_3O_4@*n*SiO_2@Al(OH)$_3$ precursors with the assistance of melamine. The catalyst with an optimum calcination temperature of 700 ℃ and theoretical Phen-Fe^{2+} loading of 6% showed the best catalytic performance in the catalytic transfer hydrogenation of halogenated nitrobenzenes. The high catalytic efficiency of the catalysts was attributed to the large specific surface area and pore size, which enabled the excellent dispersibility of Fe species and facilitated the mass transfer during the reaction process. What's more, Phen-Fe^{2+} ligands could restrict the overgrowth of Fe species and then obtain active components with smaller particle size. Mesoporous nitrogen-doped carbon layer could be introduced by the calcination of melamine and Phen, which could anchor the Fe species to avoid agglomeration or even leaching and increase the stability of the catalyst. Fe-N-C/Fe_3O_4@*n*SiO_2@Al_2O_3 catalyst can be recovered by using external magnets due to its ferromagnetism, and reused at least 7 times without significantly decrease of activity and selectivity.@Al(OH)3

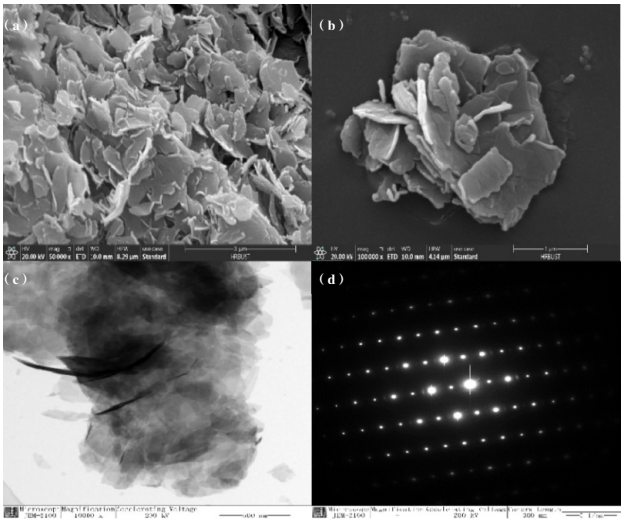


Preparation and Catalytic Properties of Inorganic Hybrid Lipase

CHEN Lin-lin, ZHANG Jia-xin, LI Wei, WANG Ling, SONG Jia-qi, XIN Jia-ying

J. Mol. Catal. (China) **2022**, 36(3): 235~244

As a commonly used biocatalyst, lipase has problems such as poor stability and difficulty in reuse. Therefore, a variety of enzyme immobilization methods have been established to improve the application of lipase. This article, based on a new method of enzyme immobilization-lipase hybrid nanoflowers formed by free lipase, we systematically study the effects of four common metal ions Ca^{2+}, Zn^{2+}, Mn^{2+}, Cu^{2+} on the secondary structure, effects of catalytic activity, tolerance and reproducibility under optimal reaction conditions. The synthesized inorganic hybrid nanoflower has a unique porous flower-like structure and a large surface area, which is conducive to the occurrence of the mass transfer process, and can also effectively improve the utilization rate of enzymes and reduce the waste of free enzymes; the synthesized immobilized enzymes it has the advantages of easy recovery and reusability, and can improve the activity and storage stability of the enzyme while reducing the use cost of the enzyme. The synthesized material metal phosphate is easy to obtain, the reaction environment is mild, and the synthesis method is green and simple, which helps to maintain the activity of the immobilized enzyme and provides a research basis for exploring the application potential of the immobilized enzyme in practice.

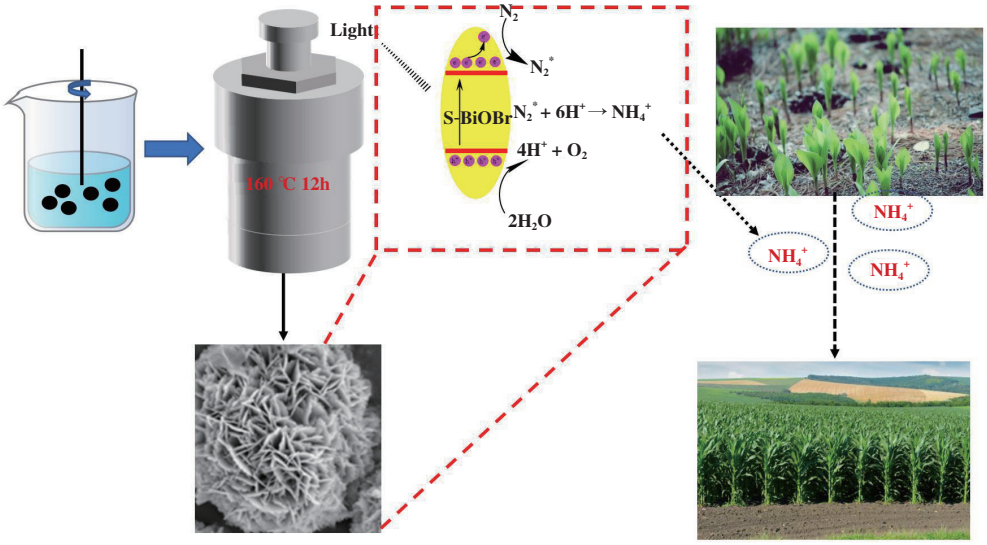


Preparation of S Doped BiOBr Photocatalyst and Its Nitrogen Fixation Performance

GE Jian-hua, ZHANG Wan, DING Xiu-long, WEI Zhou, LI Jia

J. Mol. Catal. (China) **2022**, 36(3): 245~252

Nitrogen photofixation via BiOBr-based photocatalysts have received a good deal of attentions recently. In this study, a novel S-doped BiOBr photocatalysts with were synthesized by solvothermal process. Characterization results revealed that the S-doped BiOBr photocatalyst have enhanced the nitrogen photofixation activity. It was also found that the rate of NH_4^+ production for N_2 photofixation of S-doped BiOBr is approximately ~4.6 times higher than that of bulk BiOBr. Furthermore, after four cycle experiments, the S-doped BiOBr still has high nitrogen fixation efficiency.

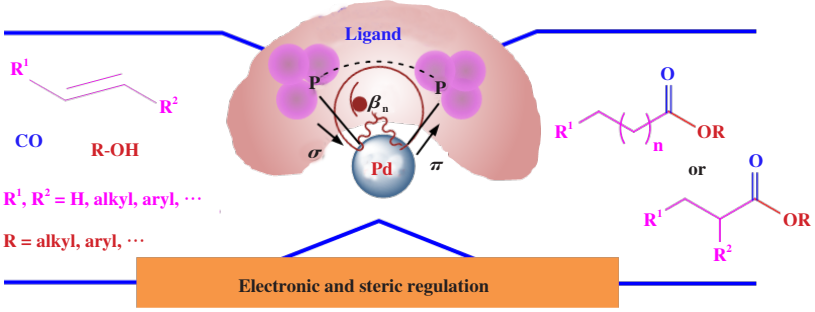


Influence of Electronic and Steric Factors of Phosphine Ligands upon Palladium-catalyzed Alkoxycarbonylation

LIU Meng-li, ZENG Bo, HU Bo, LI Zhen, XIA Chun-gu

J. Mol. Catal. (China) **2022**, 36(3): 253~273

Phosphine ligand-modified palladium catalysts are widely used in the carbonylation-esterification of unsatu-rated compounds, and their catalytic activity depends largely on the ligand environment around the metal. The variation of substituents on P atoms will regulate the steric and electronic contributions of phosphorus ligands. Many attempts have been made to quantify this ligand effect, and some ligand parameters including cone angle (θ), bite angle (β), etc, have been proposed to describe this effect quantitatively or qualitatively. Understanding the relationship of these parameters with the reactivity and selectivity will be helpful to the rational design of ligands and predicting the physical properties and catalytic activity of new catalyst systems.



Recent Advances on the Photocatalytic Regeneration of NAD(P)H

DONG Wen-jin, CHEN Fu-shan, DENG Li, XIAN Mo

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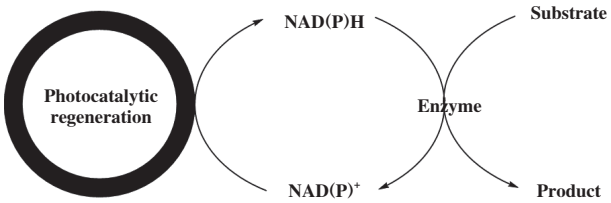
Regeneration of NAD(P)H is essential for in vitro biocatalytic synthesis because NAD(P)H are involved in most biological transformations involving enzymatic redox reactions.Among various methods, photocatalytic method has attracted more and more attention due to its utilization of abundant and clean solar energy and its mild reaction conditions.



Application and Progress of the Perovskite Materials in Environmental Catalysis

LI Chao, LI Zai-xing, CHEN Xiao-fei, ZHANG Qin-qin, MA Wei-Tao, NIU Jian-rui, XING Qian, TIAN Zhan-wei, ZHANG Chen-yang, QI Hao-jie

J. Mol. Catal. (China) **2022**, 36(3): 287~300

Nowadays, the issue of the environment is receiving ever increasing attention. Heterogeneous catalysts play an important role in environmental governance. The application of perovskite in catalysts has received extensive attention, due to its stable structure and special physical and chemical properties. The material properties, preparation methods, development status of new perovskite materials and their applications in environmental catalysis were reviewed, and the challenges and future development directions were discussed.