



## Contents

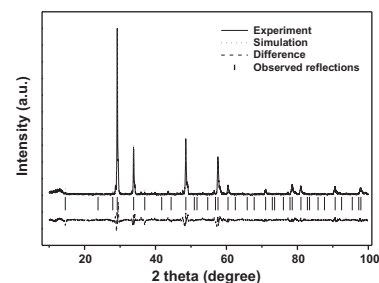
### Articles

**Jingfei Luan, Kun Ma, Bingcai Pan, Yongmei Li, Xiaoshan Wu, Zhigang Zou**

*Journal of Molecular Catalysis A: Chemical 321 (2010) 1*

Synthesis and catalytic activity of new Gd<sub>2</sub>BiSbO<sub>7</sub> and Gd<sub>2</sub>YSbO<sub>7</sub> nanocatalysts

Gd<sub>2</sub>BiSbO<sub>7</sub> and Gd<sub>2</sub>YSbO<sub>7</sub> were prepared for the first time and their structural and photocatalytic properties were investigated under visible light irradiation. The lattice parameters and band gaps of Gd<sub>2</sub>BiSbO<sub>7</sub> and Gd<sub>2</sub>YSbO<sub>7</sub> were obtained. Gd<sub>2</sub>YSbO<sub>7</sub> and Gd<sub>2</sub>BiSbO<sub>7</sub> showed higher catalytic activity for photocatalytic degradation of rhodamine B compared with Bi<sub>2</sub>InTaO<sub>7</sub>. The possible photocatalytic degradation pathway of rhodamine B was revealed.

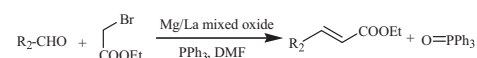


**M. Lakshmi Kantam, K.B. Shiva Kumar, V. Balasubramanyam, G.T. Venkanna, F. Figueras**

*Journal of Molecular Catalysis A: Chemical 321 (2010) 10*

One-pot Wittig reaction for the synthesis of  $\alpha$ ,  $\beta$ -unsaturated esters using highly basic magnesium/lanthanum mixed oxide

Highly basic Mg/La mixed oxide (Mg/La MO) is an effective heterogeneous base for the one-pot Wittig reaction involving aldehyde,  $\alpha$ -halo esters and triphenylphosphine to afford  $\alpha$ , $\beta$ -unsaturated esters in good yields with high *E*-stereoselectivity at room temperature. The Mg/La mixed oxide was recovered quantitatively by simple filtration and reused.

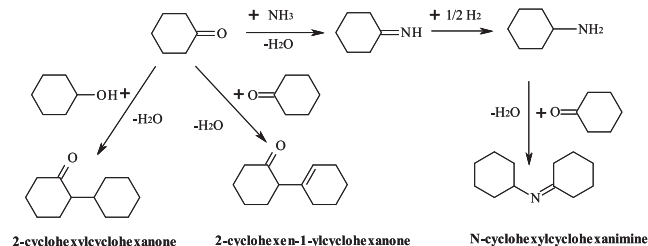


**Sharath R. Kirumakki, Maria Papadaki, Komandur V.R. Chary, N. Nagaraju**

*Journal of Molecular Catalysis A: Chemical 321 (2010) 15*

Reductive amination of cyclohexanone in the presence of cyclohexanol over zeolites H $\beta$  and HY

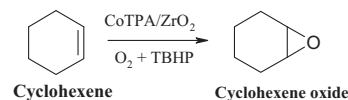
Reductive amination of a mixture of cyclohexanone/cyclohexanol in varying proportions has been carried out in gas phase over zeolites H $\beta$  and HY. The product distribution during the experiments indicates that cyclohexanol does not undergo reductive amination over acid catalysts; it only forms a condensation product with cyclohexanone. Kinetic studies during the reaction show that this reaction follows a Langmuir–Hinshelwood pathway by the adsorption of both cyclohexanone and the NH<sub>3</sub> on the surface of the zeolite. The active sites for this reaction are postulated to be the weak and moderate acid sites and not the strong acid sites on these zeolites.



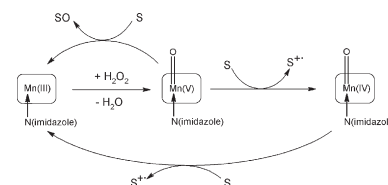
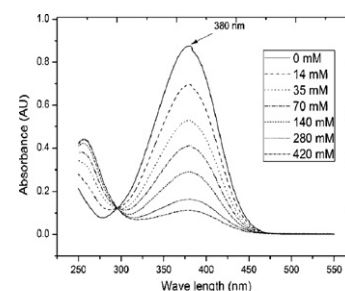
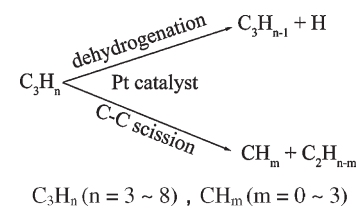
**Pragati Shringarpure, Anjali Patel***Journal of Molecular Catalysis A: Chemical* 321 (2010) 22

Cobalt (II) exchanged supported 12-tungstophosphoric acid: Synthesis, characterization and non-solvent liquid phase aerobic oxidation of alkenes

The synthesized Co exchanged supported 12-tungstophosphoric acid gives 98% conversion for the oxidation of cyclohexene with 57% selectivity for cyclohexene oxide with molecular oxygen under very mild conditions.

**Paolo Zucca, Carla Vinci, Antonio Rescigno, Emil Dumitriu, Enrico Sanjust***Journal of Molecular Catalysis A: Chemical* 321 (2010) 27

Is the bleaching of phenosafranine by hydrogen peroxide oxidation catalyzed by silica-supported 5,10,15,20-tetrakis-(sulfonatophenyl)porphine-Mn(III) really biomimetic?

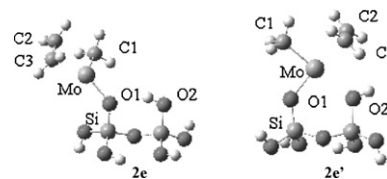
Phenosafranine degradation is reported by  $\text{H}_2\text{O}_2$  oxidation in the presence of immobilized 5,10,15,20-tetrakis(4-sulfonatophenyl)-porphine-Mn(III) catalyst. The proposed method was also compared to other bleaching methods, both chemical and enzymatic.**Kishore Kondamudi, Pandian Elavarasan, Paul J. Dyson, Sreedevi Upadhyayula***Journal of Molecular Catalysis A: Chemical* 321 (2010) 34Alkylation of *p*-cresol with *tert*-butyl alcohol using benign Brønsted acidic ionic liquid catalystBrønsted acidic ionic liquids with  $\text{SO}_3\text{-H}$  functionality were prepared, characterized and their catalytic activity in *tert*-butylation of *p*-cresol with *tert*-butyl alcohol was investigated. Kinetic investigations show lower alcohol to *p*-cresol mole ratios, lower ionic liquid to *p*-cresol ratio and temperature as low as 70 °C gave *p*-cresol conversion. The catalyst activity was retained even after 5 cycles.Absorption spectra of 4-nitroaniline for various concentrations of IL-1 in  $\text{H}_2\text{O}$ .**Ming-Lei Yang, Yi-An Zhu, Chen Fan, Zhi-Jun Sui, De Chen, Xing-Gui Zhou***Journal of Molecular Catalysis A: Chemical* 321 (2010) 42Density functional study of the chemisorption of  $\text{C}_1$ ,  $\text{C}_2$  and  $\text{C}_3$  intermediates in propane dissociation on Pt(1 1 1)The side reactions in propane dehydrogenation process yield many intermediates, including the  $\text{C}_1$ ,  $\text{C}_2$  and  $\text{C}_3$  species. This paper presents the favored adsorption configurations of all the reaction intermediates on Pt(1 1 1). Based on the adsorption energies and Brønsted-Evans-Polanyi (BEP) analysis, the energetically preferred product and favored reaction pathway can be obtained.

**Xiaochun Cao, Ruihua Cheng, Zhen Liu,  
Lisong Wang, Qi Dong, Xuelian He, Boping Liu**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 50

DFT and PIO study of the influences of Mo valance state and surface hydroxyl on supported-MoO<sub>x</sub> catalysts for ethylene polymerization

Mo<sup>2+</sup> was first found to be the most plausible active site for ethylene polymerization among catalyst models with different valence states (5+, 4+, 3+, 2+) supported on Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>, and surface hydroxyl could poison the catalyst through coordination with Mo<sup>2+</sup> center by DFT and PIO methods.

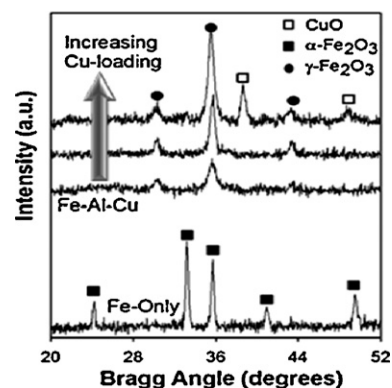


**Preshit Gawade, Burcu Mirkelamoglu, Bing Tan,  
Umit S. Ozkan**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 61

Cr-free Fe-based water-gas shift catalysts prepared through propylene oxide-assisted sol-gel technique

Cu loading in Fe-Al-Cu catalysts prepared with propylene oxide-assisted sol-gel technique may change the rate determining step in the redox mechanism. XRD shows changes in crystal phases with Cu loading.

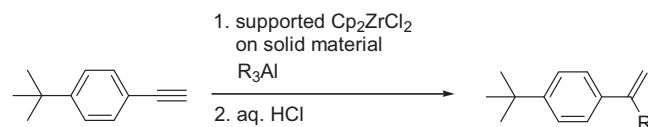


**Ryukichi Takagi, Nao Igata, Kazuhiro Yamamoto,  
Satoshi Kojima**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 71

Alkylaluminum of arylacetylene catalyzed by zirconocene catalysts supported on solid materials

The effect of using solid supporting materials in the Zr-catalyzed alkylaluminum reaction was examined. The heterogeneous system was found to be equally active as the homogeneous Cp<sub>2</sub>ZrCl<sub>2</sub>/MAO system for methylaluminum. Solvent effects in the ethylaluminum reaction suggested that the high activity of the heterogeneous systems was attributable to the delocalization of negative charge of the supporting material.

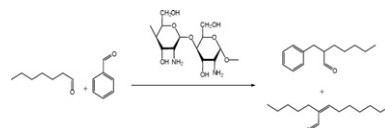


**N. Sudheesh, Sumeet K. Sharma, Ram S. Shukla**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 77

Chitosan as an eco-friendly solid base catalyst for the solvent-free synthesis of jasminaldehyde

Jasminaldehyde is a perfumery chemical of commercial interest and is synthesized under solvent-free conditions by the condensation of 1-heptanal with benzaldehyde in the presence of an eco-friendly solid base catalyst, chitosan. The condensation depended on the catalyst amount, 1-heptanal to benzaldehyde ratio, and temperature and the catalyst was recycled effectively.

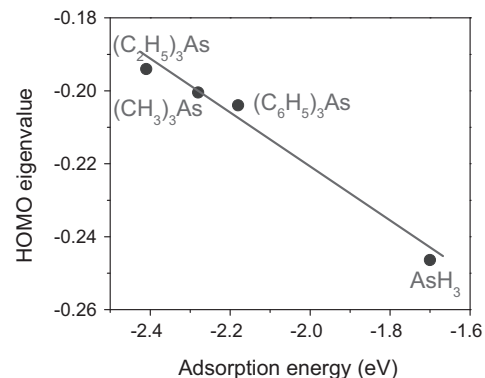


**Shaofeng Yang, John Adjaye,  
William C. McCaffrey, Alan E. Nelson**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 83

Density-functional theory (DFT) study of arsenic poisoning of NiMoS

Arsenic poisoning of NiMoS hydrotreating catalysts was studied using density-functional theory (DFT) calculations. The adsorption of organoarsenic compounds is energetically favored on both Ni(1 0 0)Mo- and Ni(1 0 0) S-edge surfaces and there is a correlation between the adsorptivity of the arsenic compounds and their electronic structure.

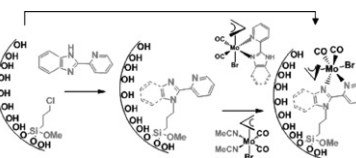


**Marta S. Saraiva, Carla D. Nunes, Teresa G. Nunes,  
Maria José Calhorda**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 92

The effect of immobilization on the catalytic activity of molybdenum  $\eta^3$ -allyldicarbonyl complexes with nitrogen donor ligands bearing N-H groups

Dicarbonyl(allyl)molybdenum complexes with pyridylimidazole ligands can be successfully immobilized in MCM-41 previously functionalized with trimethoxychlorosilane and are more active as heterogeneous catalysts for the olefin epoxidation reaction than their homogeneous congeners.

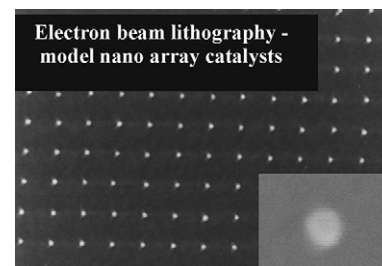


**E. Kadossov, S. Cabrini, U. Burghaus**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 101

Adsorption kinetics and dynamics of CO on silica supported Au nanoclusters—Utilizing physical vapor deposition and electron beam lithography

Physical vapor deposition and electron beam lithography have been used to study the adsorption of CO on silica supported gold clusters utilizing ultra-high vacuum kinetics and spectroscopic techniques as well as using molecular beam scattering methods.



**Habib Firouzabadi, Nasser Iranpoor,  
Mohammad Gholinejad**

*Journal of Molecular Catalysis A: Chemical* 321 (2010) 110

Recyclable palladium-catalyzed Sonogashira–Hagihara coupling of aryl halides using 2-aminophenyl diphenylphosphinite ligand in neat water under copper-free condition

An efficient copper-free Sonogashira–Hagihara reaction was performed in the presence of 2-aminophenyl diphenylphosphinite as a ligand, Pd(OAc)<sub>2</sub> and base at 25–95 °C in water under heterogeneous conditions.

