



## Contents

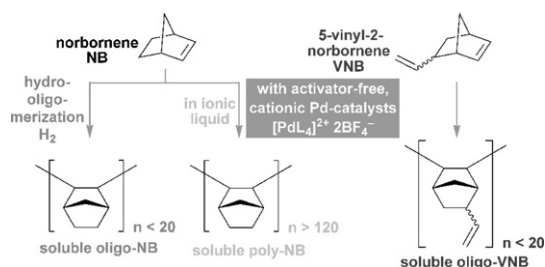
### Articles

**Frederik Blank, Harald Scherer, Christoph Janiak**

*Journal of Molecular Catalysis A: Chemical 330 (2010) 1*

Oligomers and soluble polymers from the vinyl polymerization of norbornene and 5-vinyl-2-norbornene with cationic palladium catalysts

Hydrooligomerization, an ionic liquid as solvent and a norbornene derivative with an  $\alpha$ -olefin functionality leads to oligonorbornene, soluble polynorbornene (PNB), and oligo (5-vinyl-2-norbornene) (oligo-VNB), respectively, with cationic palladium catalysts.

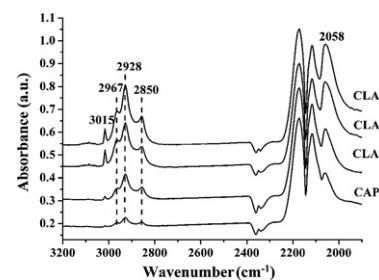


**Zhe Cai, Jinlin Li, Kongyong Liew, Juncheng Hu**

*Journal of Molecular Catalysis A: Chemical 330 (2010) 18*

Effect of  $\text{La}_2\text{O}_3$ -dopping on the  $\text{Al}_2\text{O}_3$  supported cobalt catalyst for Fischer-Tropsch synthesis

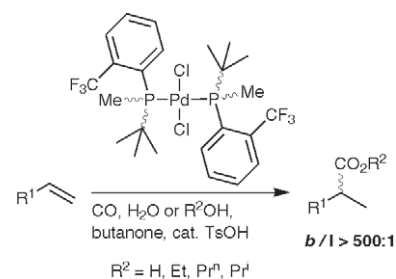
The DRIFTS spectra of syngas adsorbed on reduced catalysts were collected at 503 K. The new peak located at  $2058\text{ cm}^{-1}$  is not only directly related to the bands of hydrocarbon ( $2800\text{--}3100\text{ cm}^{-1}$ ), but also related to CO conversion and chain-growth. This peak is ascribed to the "hydrocarbonyl" species, may be a vibrational feature of some reaction intermediate.



**Arnald Grabulosa, Jamie J.R. Frew, José A. Fuentes, Alexandra M.Z. Slawin, Matthew L. Clarke**

*Journal of Molecular Catalysis A: Chemical 330 (2010) 18*

Palladium complexes of bulky *ortho*-trifluoromethylphenyl-substituted phosphines: Unusually regioselective catalysts for the hydroxycarbonylation and alkoxy carbonylation of alkenes

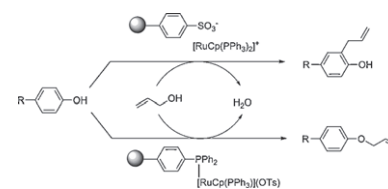


**Jimmy A. van Rijn, Elisabeth Bouwman, Eite Drent**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 26

Immobilization of ruthenium catalysts for allylations with allyl alcohol

Immobilization of  $[\text{RuCp}(\text{PP})]^+$  complexes was achieved via electrostatic or coordination interactions. In the catalytic allylation of phenol the selectivity is dependent on the method used for immobilization of the catalyst.

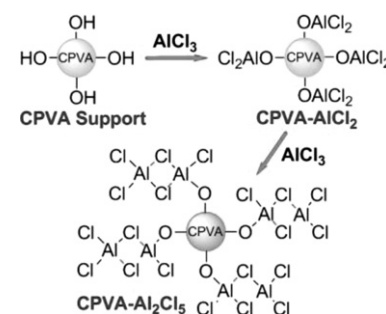


**Zhanbin Wang, Baojiao Gao**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 35

Preparation, structure, and catalytic activity of aluminum chloride immobilized on cross-linked polyvinyl alcohol microspheres

$\text{AlCl}_3$  was covalently bound onto cross-linked polyvinyl alcohol (CPVA) microspheres, obtaining an immobilized Lewis acid catalyst CPVA- $\text{AlCl}_3$ . During the immobilization reaction, the structure of bound  $\text{AlCl}_3$  gradually changed from the monomeric form ( $-\text{AlCl}_2$ ) to the dimeric form ( $-\text{Al}_2\text{Cl}_5$ ), which gave rise to a catalytic activity enhancement.

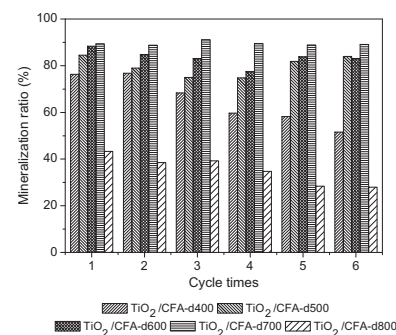


**Jian-wen Shi, Shao-hua Chen, Shu-mei Wang, Zhi-long Ye, Peng Wu, Bin Xu**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 41

Favorable recycling photocatalyst  $\text{TiO}_2/\text{CFA}$ : Effects of calcination temperature on the structural property and photocatalytic activity

The  $\text{TiO}_2/\text{CFA-d700}$  was the optimal photocatalyst among all samples because a high mineralization ratio was always maintained without any decline when it was used repeatedly, even at the sixth cycle.

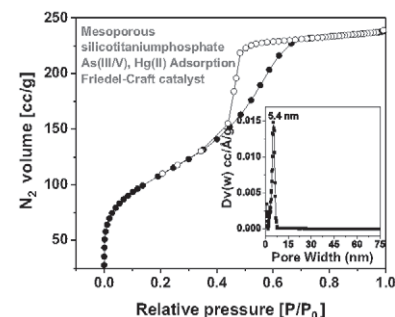


**Manidipa Paul, Nabanita Pal, M. Ali, Asim Bhaumik**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 49

New mesoporous silicotitaniumphosphate and its application in acid catalysis and adsorption of As(III/V), Cd(II) and Hg(II)

A new mesoporous silicotitaniumphosphate material has been synthesized by using Pluronic F127 as template, which showed high catalytic activity in Friedel-Craft benzylation reactions and adsorption of As(III/V) and Hg(II).

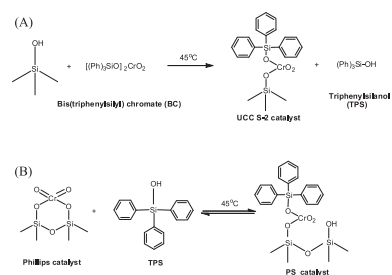


**Xiaofang Li, Ruihua Cheng, Jun Luo, Qi Dong, Xuelian He, Liuzhong Li, Yongling Yu, Jianwen Da, Boping Liu**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 56

Experimental and theoretical studies on ethylene polymerization using SiO<sub>2</sub>-supported silyl chromate type catalysts prepared by a green method

A green route for preparation of SiO<sub>2</sub>-supported silyl chromate type catalysts through transformation from Phillips catalyst by reaction with triphenylsilanol (TPS) without using toxic bis(triphenylsilyl) chromate was investigated by theoretical and experimental methods.

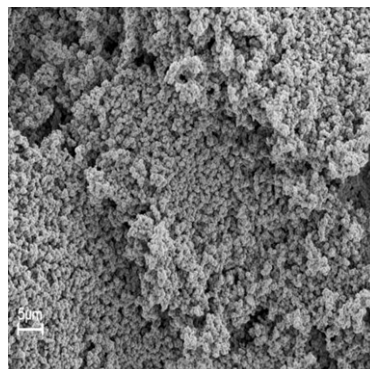


**Hariharaputhiran Subramanian, Elizabeth G. Nettleton, Sridhar Budhi, Ranjit T. Koodali**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 66

Baeyer–Villiger oxidation of cyclic ketones using Fe containing MCM-48 cubic mesoporous materials

Fe-MCM-48 mesoporous materials were prepared at room temperature and characterized by a variety of techniques. These materials exhibited high catalytic activity towards the Baeyer–Villiger oxidation of cyclic ketones.

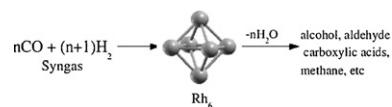


**Sharan Shetty, Rutger A. van Santen, Paul A. Stevens, Sumathy Raman**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 73

Molecular steps for the syngas conversion on the Rh<sub>6</sub> cluster

In the present theoretical study we use density functional approach to investigate the reaction pathways of the elementary steps involved in the syngas conversion leading to C<sub>1</sub>, C<sub>2</sub> oxygenated compounds, methane and water on Rh<sub>6</sub> cluster.

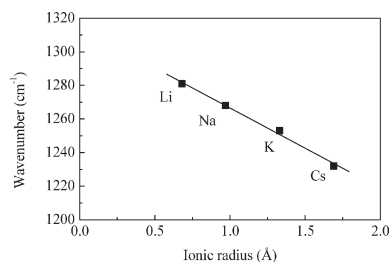


**Ruth L. Martins, Claudia de O. Veloso, Claudio A. Mota, Martin Schmal**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 88

Infrared spectroscopic characterization of basic properties: Nitromethane as probe molecule

Nitromethane, as probe molecule, and infrared spectroscopy were used to characterize basic properties of alkali-exchanged X zeolites and metal oxides. On zeolites the rock angular bending band was sensitive to the electrostatic field produced by the alkali cation and its frequency varies linearly with the ionic radius of the cation.

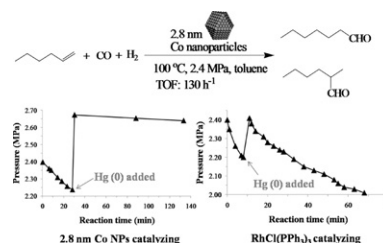


**Zhipeng Cai, Hang Wang, Chaoxian Xiao,  
Mengqi Zhong, Ding Ma, Yuan Kou**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 94

Hydroformylation of 1-hexene over ultrafine cobalt nanoparticle catalysts

2.8 nm cobalt nanoparticles were prepared to catalyze hydroformylation of 1-hexene under low pressure and mercury poisoning test suggest a heterogeneous catalysis mechanism for the system.

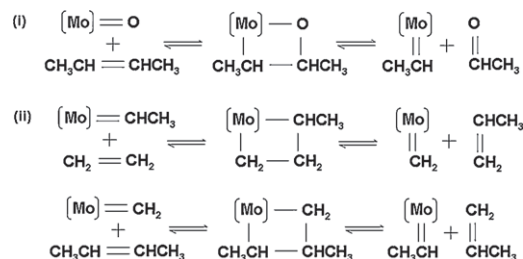


**Xin Li, Jing Guan, Anmin Zheng, Danhong Zhou,  
Xiuwen Han, Weiping Zhang, Xinhe Bao**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 99

DFT studies on the reaction mechanism of cross-metathesis of ethylene and 2-butylene to propylene over heterogeneous Mo/HBeta catalyst

DFT calculations on the reaction mechanism of olefin metathesis reveal that Mo<sup>V</sup>-carbenes are more preferred to be the active sites, which is consistent with experimental findings.

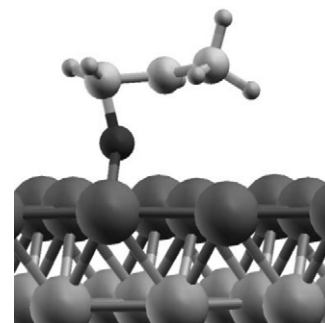


**Ali Can Kizilkaya, Selim Senkan, Isik Onal**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 107

Investigation of ruthenium-copper bimetallic catalysts for direct epoxidation of propylene: A DFT study

Propylene epoxidation reactions are carried out on Ru-Cu(111) bimetallic surface with periodic DFT calculations. Ru-Cu(111) surface is ineffective for epoxidation due to the high basicity of the chemisorbed oxygen atom.



**Ali Nakhaei Pour, Mohammad Reza Housaindokht,  
Sayyed Faramarz Tayyari, Jamshid Zarkesh,  
Mohammad Reza Alaei**

*Journal of Molecular Catalysis A: Chemical* 330 (2010) 112

Deactivation studies of Fischer-Tropsch synthesis on nano-structured iron catalyst

Deactivation kinetics of bulk and nanostructured microemulsion prepared iron catalysts were studied in Fischer-Tropsch synthesis (FTS), from fitting of data to a generalized power-law expression (GPLE),  $r_d = k_d (a - a_{\infty})^m$ .

