



Journal of Molecular Catalysis A: Chemical 279 (2008) v-ix

www.elsevier.com/locate/molcata

## Contents

#### Articles Matthew M. Yung, Zhongkui Zhao, Matthew Cobalt oxide supported on zirconia was tested for P. Woods, Umit S. Ozkan the preferential oxidation of CO in excess H2 under H<sub>2</sub>O a variety of conditions. High O2 selectivity was achieved at T < 200 °C. At higher temperatures, H<sub>2</sub> Journal of Molecular Catalysis A: Chemical 279 (2008) 1 combustion and methanation became important. The figure shows temperature-programmed reaction [a.u.] CH/ Preferential oxidation of carbon monoxide on over CoO<sub>x</sub>/ZrO<sub>2</sub> in the presence of 1% CO, 1% O<sub>2</sub>, Intensity 60% H<sub>2</sub>, balance He. $C_0O_y/Z_TO_2$ co co₂ O2 175 225 275 Hold at 300°C (30 min) 75 125 25

#### Mika Kobune, Satoshi Sato, Ryoji Takahashi

Journal of Molecular Catalysis A: Chemical 279 (2008) 10

Surface-structure sensitivity of  ${\rm CeO}_2$  for several catalytic reactions

Vapor-phase reactions of several reactants were investigated over  $CeO_2$  catalysts with different particle sizes, and the surface-structure sensitivity was discussed.  $CeO_2$  {1 1 1} facets have active sites for the reactions of butanediols and of propanoic acid, which can be categorized into structure-sensitive reaction. The structure-sensitive reactions have feature that the main product(s) are formed with high selectivity at temperatures lower than 400 °C.



#### Ming-Show Wong, Shih-Wei Hsu, K. Koteswara Rao, Chinthala Praveen Kumar

Journal of Molecular Catalysis A: Chemical 279 (2008) 20

Influence of crystallinity and carbon content on visible light photocatalysis of carbon doped titania thin films

Department of Materials Science and Engineering, National Dong Hwa University, Hualien-974, Taiwan, ROC Carbon doped  $\text{TiO}_2$  films were developed by ion-assisted electron-beam evaporation. Post annealing at a higher temperature improved the film crystallinity. This work demonstrates clearly that the photocatalytic performance of the  $\text{TiO}_x C_y$ films under visible light correlates well with the anatase crystallinity and carbon dopant concentration. The SEM images show silver metal particles photo-reduced on carbon-doped titania films before (left) and after annealing (right).



Temperature I°C1

Hiroyoshi Maekawa, Tomoko Shibata, Akita Niimi, Chiharu Asaoka, Kaori Yamasaki, Hiroaki Naiki, Kenichi Komura, Yoshihiro Kubota, Yoshihiro Sugi, Jae-Youl Lee, Jong-Ho Kim, Gon Seo

Journal of Molecular Catalysis A: Chemical 279 (2008) 27

The isopropylation of biphenyl over one-dimensional zeolites with corrugated channels

The isopropylation of biphenyl was examined over one-dimensional zeolites with corrugated channels: SSZ-55, SSZ-42, L, and SSZ-35 zeolites. The selectivities for 4,4'-diisopropylbiphenyl (4,4'-DIPB) over these zeolites were 10–40%: they are much lower than that of MOR in spite of similar size of pore-entrance. They have larger reaction spaces than MOR due to their corrugated channels. They are too large for the selective formation of 4,4'-DIPB.



#### Joyanta Choudhury, Sujit Roy

Journal of Molecular Catalysis A: Chemical 279 (2008) 37

Ir/Sn dual reagent catalysis for the alkylation of arenes with benzyl alcohols: Kinetic evidence for an electrophilic pathway and a guide towards electronic tuning of catalyst efficiency The alkylation of arene/heteroarene with benzyl alcohols is efficiently catalyzed by  $[Ir(COD)(\mu-Cl)]_2/SnCl_4$  dual-catalyst. A working model on substrate activation across Ir/Sn catalyst is proposed based on HSAB consideration. Kinetic evidences support an electrophilic mechanism, absence of a C–H activation pathway and similarity with Friedel–Crafts like kinetics. The stereoelectronic influence of the metal centers on catalyst efficiency is also studied.





#### A. Knapik, A. Drelinkiewicz, M. Szaleniec, W. Makowski, A. Waksmundzka-Góra, A. Bukowska, W. Bukowski, J. Noworól

Journal of Molecular Catalysis A: Chemical 279 (2008) 47

Hydrogenation of unsaturated carboxylic acids on functional gel-type resin supported Pd catalysts: The effect of reactant structure Functional gel-type resin-based Pd catalysts (0.5–2 wt.% Pd) of well dispersed Pd nanoparticles were prepared and characterized by SEM, TEM techniques, swelling and porosity measurements. The role of specific properties of functional gel-type matrix in the Pd catalysts was studied in the hydrogenation of unsaturated carboxylic acids, derivatives of acrylic acid. The role of the size of the substrate molecule, its hydrophobicity and absolute hardness/polarizability in the rate of C=C hydrogenation has been established by theoretical modelling.



#### U.B. Demirci, F. Garin

Journal of Molecular Catalysis A: Chemical 279 (2008) 57

Kinetics of Ru-promoted sulphated zirconia catalysed hydrogen generation by hydrolysis of sodium tetrahydroborate

Hydrogen can be catalytically generated by hydrolysis of sodium tetrahydroborate NaBH<sub>4</sub>. The kinetic data (reaction orders and apparent activation energy) of this hydrolysis reaction were determined for 1 wt% Ru-promoted sulphated zirconia. The established hydrogen generation rate can be given following a power law:  $r = k[\text{NaBH}_4]^{0.23}[\text{NaOH}]^{-0.35}[\text{Ru}]^{1.27}$  with  $k = A \exp(-76.10^3/RT)$ .



#### P.F. Siril, H.E. Cross, D.R. Brown

Journal of Molecular Catalysis A: Chemical 279 (2008) 63

New polystyrene sulfonic acid resin catalysts with enhanced acidic and catalytic properties The effects of halogenation of polystyrene sulfonic acid resins on acidic and catalytic properties have been evaluated.



#### Chen Xu, Jun-Fang Gong, Tao Guo, Yan-Hui Zhang, Yang-Jie Wu

Two stable cyclopalladated ferrocenylimine complexes with monophosphinobiphenyl ligands **4** and **5** have been easily synthesized and structurally characterized. Single crystal X-ray analysis revealed the *anti*, *trans*-structure of palladacycle **4** as well as the *syn*, *trans*-structure of **5** in the solid state. The two complexes could effectively catalyze the Suzuki reaction of various aryl chlorides and phenylboronic acid.

Journal of Molecular Catalysis A: Chemical 279 (2008) 69

Cyclopalladated ferrocenylimine complexes with dicyclohexylphosphinobiphenyl ligands: Synthesis, crystal structures and their use as highly efficient catalysts for Suzuki reaction of aryl chlorides



#### Yue-hua Xu, Zhuo-xian Zeng

Journal of Molecular Catalysis A: Chemical 279 (2008) 77

The preparation, characterization, and photocatalytic activities of Ce-TiO<sub>2</sub>/SiO<sub>2</sub>

The high photocatalytic activity of Ce-TiO<sub>2</sub>/SiO<sub>2</sub> can be explained by the effective separation of photogenerated electron-hole pairs, which are trapped by Ce<sup>4+</sup> and hydroxyl groups balancing the positive charge generated by the incorporation of Si in a Ti matrix, respectively.



#### Tao Zhang, Jun Ma

Journal of Molecular Catalysis A: Chemical 279 (2008) 82

Catalytic ozonation of trace nitrobenzene in water with synthetic goethite

This work aimed to reveal the mechanisms of catalytic ozonation of a refractory pollutant (nitrobenzene) with synthetic goethite (FeOOH) in water. Results revealed that zero-charged surface hydroxyl groups on FeOOH in water are the active sites in inducing ozone decomposition to generate hydroxyl radicals during the enhanced oxidation of the pollutant that can not form surface complexes with the catalyst.



#### Tao Jiang, Sai Zhang, Xingliang Jiang, Chaofeng Yang, Bo Niu, Yingnan Ning

Journal of Molecular Catalysis A: Chemical 279 (2008) 90

The effect of *N*-aryl bisphosphineamine ligands on the selective ethylene tetramerization

A systematic study was conducted on the Cr catalyzed tetramerization of ethylene using bis(diphenylphosphino)amine ligands with *N*-aryl functionality. This study revealed that the oligomerization reaction product selectivity is primarily dependent on the structure and size of the *N*-aryl groups. Activated by methylaluminoxane, the best ligand with 3,5-dimethylphenyl attached to N atom achieved selectivity as high as 86.13% (1-octene and 1-hexene) and catalytic activity up to  $4.98 \times 10^6$  g/mol Cr h. It was concluded that structural fine tuning of the *N*-aryl moiety of the PNP ligand is essential for obtaining efficient catalysts for ethylene tetramerization toward 1-octene.

### Fabian Jutz, Jan-Dierk Grunwaldt, Alfons Baiker

Journal of Molecular Catalysis A: Chemical 279 (2008) 94

Mn(III)(salen)-catalyzed synthesis of cyclic organic carbonates from propylene and styrene oxide in "supercritical"  $CO_2$ 

Various homogeneous and immobilized manganesesalen complexes were employed as catalysts for the formation of cyclic organic carbonates from two liquid epoxides (propylene oxide and styrene oxide) and CO<sub>2</sub>, which served as reactant and solvent. Extensive parametric studies, accompanied by view cell observations and ATR-IR spectroscopy, led to an optimization of this process and revealed a complex phase behaviour dependency.



 $P(Ph)_2$ 

 $(Ph)_2P$ 

#### K.M. Parida, Sujata Mallick

Journal of Molecular Catalysis A: Chemical 279 (2008) 104

Hydroxylation of phenol over molybdovanadophosphoric acid modified zirconia



Molybdovanadophosphoric acids supported zirconia (ZMVPA) is an efficient catalyst for phenol oxidation



#### Ajjarapu Ratnamala, Kannekanti Lalitha, Jakkidi Krishna Reddy, Valluri Durga Kumari, Machiraju Subrahmanyam

Journal of Molecular Catalysis A: Chemical 279 (2008) 112

Selective vapor phase synthesis of 1,2,3,4,5,6,7,8octahydro acridin 9-ylamine over Al-MCM-41 molecular sieves Cyclization of cyclohexanone, formamide and ammonia in vapor phase gives 1,2,3,4,5,6,7,8-octahydro acridin 9-ylamine (AOHA) over zeolites HY, HZSM-5, H $\beta$  and mesoporous Al–MCM-41

molecular sieves. Co<sup>2+</sup> ion modification of Al–MCM-41 resulted into two sets of acid sites, which resulted in 100% cyclization activity facilitating the maximum synthesis of AOHA.



# J. Salomé, C. Bachmann, K. De Oliveira-Vigier, S. Brunet, J. Lopez

Journal of Molecular Catalysis A: Chemical 279 (2008) 119

Effect of the experimental conditions in the transformation of the bis-1,3-trichloromethylbenzene in the presence of HF and a Lewis acid The transformation of the bis-1,3-trichloromethylbenzene depends on the experimental conditions (temperature, amount of HF and Lewis acid). The formation of the 1-trichloromethyl-3-trifluoromethylbenzene is favored in the presence of HF in default. The presence of a Lewis acid increases the formation of the more stable products at lower temperature.



This paper demonstrates for the first time the feasibility of the highly selective and stable benzene alkylation with ethane into ethylbenzene over bifunctional zeolite catalysts and indicates the reaction conditions and catalysts for further research into this interesting and potentially important reaction.



#### Patcharaporn Weerachawanasak, Piyasan Praserthdam, Masahiko Arai, Joongjai Panpranot

Dmitry B. Lukyanov, Tanya Vazhnova

(2008) 128

PtH-MFI catalysts

Journal of Molecular Catalysis A: Chemical 279

Highly selective and stable alkylation of benzene

with ethane into ethylbenzene over bifunctional

Journal of Molecular Catalysis A: Chemical 279 (2008) 133

A comparative study of strong metal–support interaction and catalytic behavior of Pd catalysts supported on micron- and nano-sized  $\text{TiO}_2$  in liquid-phase selective hydrogenation of phenylacetylene

Reduction by  $H_2$  at 500 °C resulted in strong metal–support interaction for the nano-sized TiO<sub>2</sub> supported Pd catalyst, but not for the micron-sized TiO<sub>2</sub> supported one. The SMSI effect, however, appeared to be necessary for high catalytic performance of the Pd/TiO<sub>2</sub> catalysts in the liquid-phase selective hydrogenation of phenylacetylene to styrene.



#### Yan Li, Zhen-Guo Li, Ren-Xian Zhou

Journal of Molecular Catalysis A: Chemical 279 (2008) 140

Bimetallic Pt-Co catalysis on carbon nanotubes for the selective hydrogenation of cinnamaldehyde to cinnamyl alcohol: Preparation and characterization H2-TPR profiles of the CNTs supported Pt-Co catalysts are shown in Fig. 2. The Pt-Co/CNTs (I) catalyst presents a large peak of H2 consumption appearing at a higher temperature, 250 °C. The high consumption of H2 (H2/Pt = 3.3) is in accordance with that already observed and can be interpreted by the following equation:  $\left[ Pt(OH)_4(Cl)_2 \right]^{2-} +3H2 \rightarrow Pt^0 + 4H_2O + 2HCl + 2e^-$ .The other catalysts present a reduction maximum at about 20 °C, with a H2/Pt ratio basically equal to 2.

