

## Contents

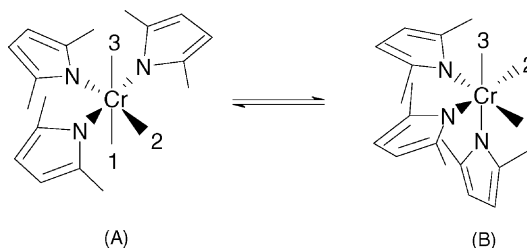
### Articles

#### He-Kuan Luo, Da-Gang Li, Song Li

*Journal of Molecular Catalysis A: Chemical 221 (2004) 9*

The effect of halide and the coordination geometry of chromium center in homogeneous catalyst system for ethylene trimerization

Facial coordination geometry (B) is much more favorable for ethylene trimerization than meridional coordination geometry (A). The promotion effect of halide component could be interpreted well from its stabilization on facial geometry (B) through the coordination of halo group with chromium center. Under the guide of this interpretation, a new catalyst system [Cr(2EH)<sub>3</sub>/2,5-dimethylpyrrole/AlEt<sub>3</sub>/2-fluoro-6-chloro- $\alpha$ ,  $\alpha$ ,  $\alpha$ -trichlorotoluene] was found demonstrating both high selectivity and activity.

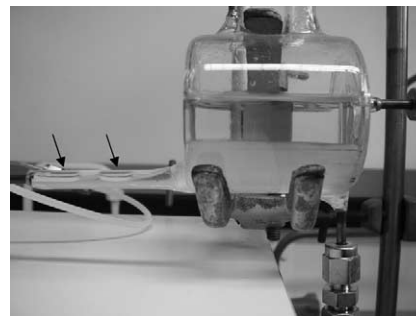


#### Evangelia Perperi, Yulin Huang, Panagiota Angeli, George Manos, David J. Cole-Hamilton

*Journal of Molecular Catalysis A: Chemical 221 (2004) 19*

Separation studies in a continuous flow fluoruous biphasic system. Proof of concept

A proof of concept study was undertaken for the separation of the fluoruous solvent from the organic reactants/products of a fluoruous biphasic system, in the absence of fluoruous modified Rh catalyst. Fast and efficient separation of the two phases was observed. The more polar products were present in the organic phase—i.e. the higher the simulated conversion level—the less was the leaching of the fluoruous solvent in the organic phase.

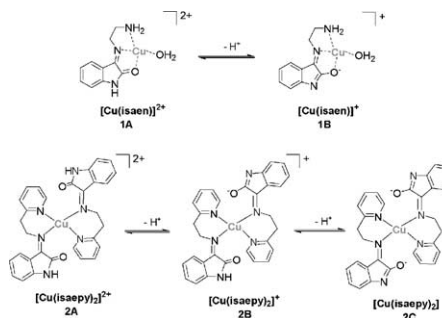


#### Giselle Cerchiaro, Gustavo A. Micke, Marina Franco Maggi Tavares, Ana Maria da Costa Ferreira

*Journal of Molecular Catalysis A: Chemical 221 (2004) 29*

Kinetic studies of carbohydrate oxidation catalyzed by novel isatin–Schiff base copper(II) complexes

With the aim of elucidating the mechanism of oxidative processes initiated by copper(II)–carbohydrate interactions, new isatin–Schiff base copper(II) complexes were isolated, and characterized by elemental analyses, UV/Vis, FTIR, EPR, and molar conductivity measurements. These complexes show keto-enolic equilibria, and had their catalytic activity in the oxidation of common carbohydrates by molecular oxygen compared.

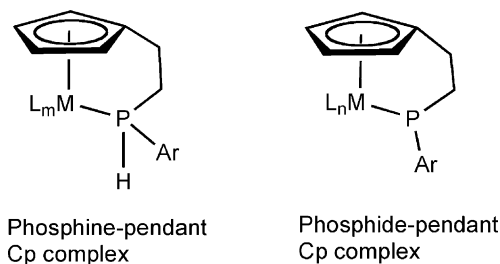


**Takeshi Ishiyama, Katsuhiko Miyoshi, Hiroshi Nakazawa**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 41

Ethylene polymerization and ethylene/styrene copolymerization with secondary phosphine-pendant and phosphide-pendant complexes of Zr and Hf

The catalytic systems obtained by a combination of zirconium or hafnium complexes bearing a secondary phosphine-pendant cyclopentadienyl ligand or a phosphide-pendant cyclopentadienyl ligand with a cocatalyst show moderate activity in ethylene polymerization but show inactivity in styrene polymerization. In ethylene/styrene copolymerization, these systems afford ethylene/styrene copolymers with a high styrene content.

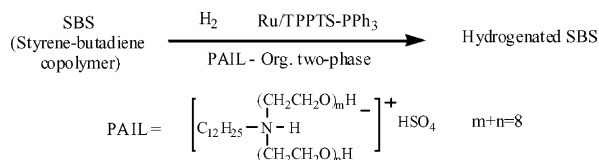


**Li Wei, Jingyang Jiang, Yanhua Wang, Zilin Jin**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 47

Selective hydrogenation of SBS catalyzed by Ru/TPPTS complex in polyether modified ammonium salt ionic liquid

The hydrogenation of SBS was carried out with a Ru/TPPTS-PPh<sub>3</sub> complex in polyether modified ammonium salt ionic liquid (PAIL) two-phase media. The catalyst can be recovered by simple phase separation and recycled three times without significant changes in the catalytic activity.

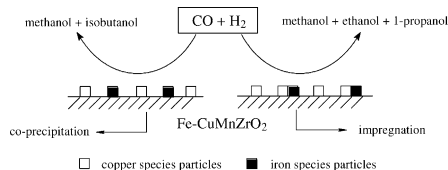


**Run Xu, Cheng Yang, Wei Wei, Wen-huai Li, Yu-han Sun, Tian-dou Hu**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 51

Fe-modified CuMnZrO<sub>2</sub> catalysts for higher alcohols synthesis from syngas

The presence of iron in CuMnZrO<sub>2</sub> catalyst resulted in substantial changes in both structure properties and catalytic performance. The dispersion of copper increased and the catalyst stabilization was improved. The role of iron was greatly influenced by catalyst preparation methods. For the Fe-CuMnZrO<sub>2</sub> catalyst prepared by co-precipitation method, iron species acted as structural promoter, which increased copper dispersion and improved the formation the homogeneous copper phase. As a result, the introduction of iron by co-precipitation method was favorable to synthesis of methanol and branched products. For the catalyst prepared by wetness impregnation method, the iron oxide-support interaction was relatively weak. The iron oxide could be partially reduced, which led to increase of the interaction between highly dispersed copper and iron. Such interaction was in favor of carbon chain growth to form higher alcohols.

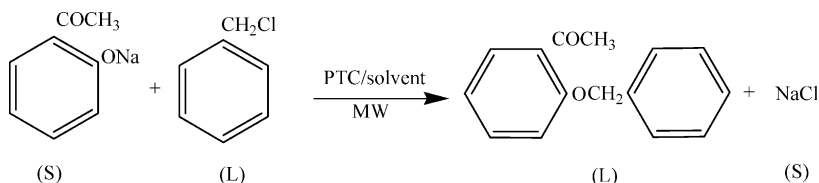


**Ganapati D. Yadav, Priyal M. Bisht**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 59

Novelties of microwave irradiated solid-liquid phase transfer catalysis (MISL-PTC) in synthesis of 2'-benzyloxyacetophenone

The microwave assisted solid-liquid PTC reaction is 100% selective with very high rates of reactions at low power inputs, and a new theory is proposed to measure simultaneously measurement of rate constant and ion exchange equilibrium constant including Gibbs free energy for the solid dissolution with anion exchange reaction.

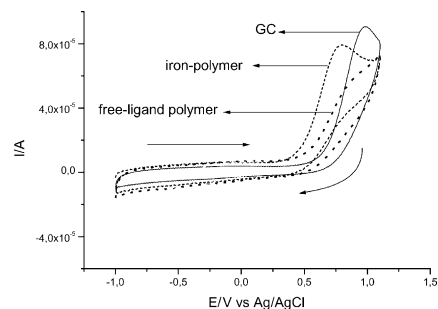


**M. Lucero, G. Ramírez, A. Riquelme, I. Azocar, M. Isaacs, F. Armijo, J.E. Förster, E. Trollund, M.J. Aguirre, D. Lexa**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 71

Electrocatalytic oxidation of sulfite at polymeric iron tetra (4-aminophenyl) porphyrin—modified electrode

An over-oxidized polymer of Fe-(III)-para-tetra-aminophenylporphyrin-glassy carbon electrode was studied as an electrocatalyst for the oxidation of sulfite. The modified electrode operates in a wide range of pH. It is very stable and can be used more than 500 consecutive cycles. The only detected product of the oxidation was sulfate. A linear relationship between the oxidation current and the sulfite concentration was founded at concentrations lower than 0.05 M.

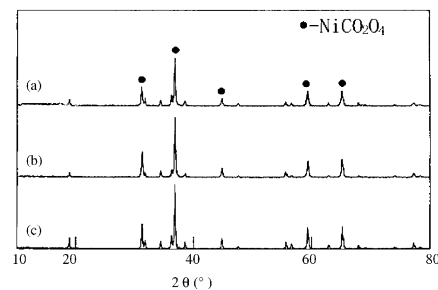


**Min Chen, Xiao-Ming Zheng**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 77

The effect of K and Al over NiCo<sub>2</sub>O<sub>4</sub> catalyst on its character and catalytic oxidation of VOCs

Potassium as additive considerably improved the activity of NiCo<sub>2</sub>O<sub>4</sub> in the total oxidation of VOCs. The typical properties and the effect of K and Al over NiCo<sub>2</sub>O<sub>4</sub> catalyst were investigated by XRD, TPR, BET and XPS technologies. The small particle size of NiCo<sub>2</sub>O<sub>4</sub> was the active sites for VOCs oxidation.

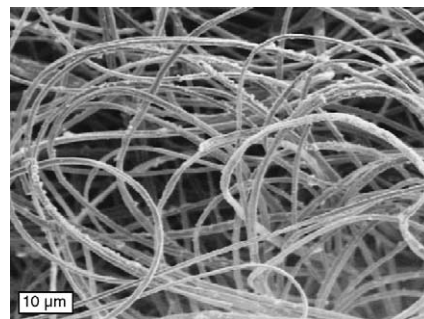


**Pingfeng Fu, Yong Luan, Xuegang Dai**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 81

Preparation of activated carbon fibers supported TiO<sub>2</sub> photocatalyst and evaluation of its photocatalytic reactivity

Activated carbon fibers supported TiO<sub>2</sub> photocatalyst, prepared by a molecular adsorption–deposition method, had a TiO<sub>2</sub> coating thickness of about 100 nm and the unfilled space between adjacent fibers. The pure anatase crystalline structure and large surface area of the immobilized photocatalyst led to efficient photodegradation of methylene blue solution.

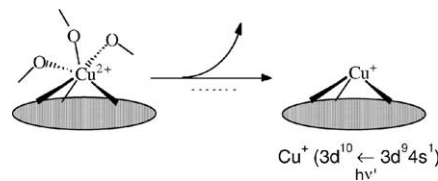


**Fumiaki Amano, Tsunehiro Tanaka, Takuzo Funabiki**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 89

Auto-reduction of Cu(II) species supported on Al<sub>2</sub>O<sub>3</sub> to Cu(I) by thermovacuum treatment

On the  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> surface, the isolated Cu<sup>2+</sup> species are easily reduced to Cu<sup>+</sup> ions by thermovacuum treatment. On the other hand, the less dispersed Cu<sup>2+</sup> species cannot be fully reduced to Cu<sup>+</sup> ions under vacuum at 973 K. The degree of the Cu dispersion determines the auto-reducibility of Cu<sup>2+</sup>/Al<sub>2</sub>O<sub>3</sub> catalysts as a whole.

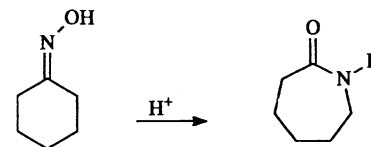


**L. Forni, C. Tosi, G. Fornasari, F. Trifirò, A. Vaccari, J.B. Nagy**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 97

Vapour-phase Beckmann rearrangement of cyclohexanone-oxime over Al-MCM-41 type meso-structured catalysts

Vapour phase Beckmann rearrangement of cyclohexanone-oxime to caprolactam has been studied using mesoporous compounds (MCM-41) with different Si/Al ratio. The use of different weight hourly space velocity (WHSV) and polar solvents has been described.

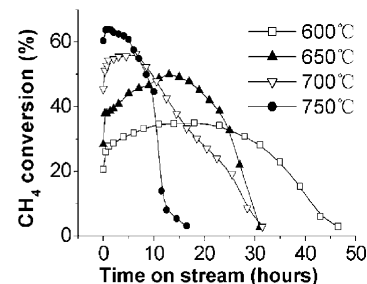


**Jianzhong Li, Gongxuan Lu, Ke Li, Weiping Wang**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 105

Active Nb<sub>2</sub>O<sub>5</sub>-supported nickel and nickel-copper catalysts for methane decomposition to hydrogen and filamentous carbon

The addition of Nb<sub>2</sub>O<sub>5</sub> changes the morphology in oxidized state and increases the relative intensity of Ni(1 1 1) planes in reduced state for Ni-Cu bimetallic catalysts. Thus, the addition of Nb<sub>2</sub>O<sub>5</sub> increases the hydrogen yield and prolongs the lifetime of bimetallic Ni-Cu catalysts in methane decomposition, especially at high temperature.

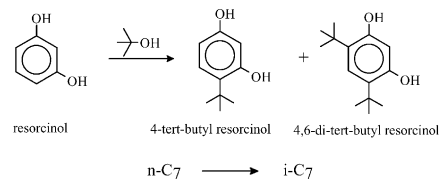


**Biju. M. Devassy, S.B. Halligudi, S.P. Elangovan, S. Ernst, M. Hartmann, F. Lefebvre**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 113

Zirconia supported phosphotungstic acid as an efficient catalyst for resorcinol *tert*-butylation and *n*-heptane hydroisomerization

The liquid-phase alkylation of resorcinol with *tert*-butanol was carried over zirconia supported PTA calcined at 750 °C as catalysts and under the optimized reaction conditions, 15% PTA gave 93.3% resorcinol conversion with selectivities to 4-*tert*-butyl resorcinol (38.8%) and 4,6-*di-tert*-butyl resorcinol (60.5%). Pt and/or Pd supported on 15% catalyst was used in *n*-heptane hydroisomerization and the one prepared from acetylacetonate complexes were more active than amine complexes.

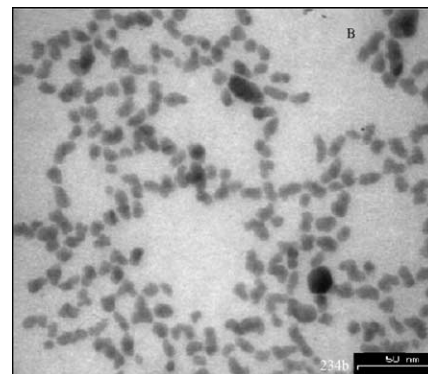


**Baolin He, Juei Juei Tan, Kong Yong Liew, Hanfan Liu**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 121

Synthesis of size controlled Ag nanoparticles

Parameters for the synthesis of size controlled and stabilized Ag nanoparticles by conventional heating and microwave methods have been determined.

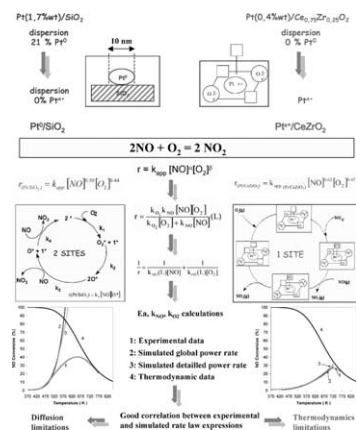


**Rui Marques, Pierre Darcy, Patrick Da Costa, Henry Mellottée, Jean-Michel Trichard, Gérald Djéga-Mariadassou**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 127

Kinetics and mechanism of steady-state catalytic NO + O<sub>2</sub> reactions on Pt/SiO<sub>2</sub> and Pt/CeZrO<sub>2</sub>

The kinetics of NO oxidation was performed over Pt<sup>0</sup>/SiO<sub>2</sub> Pt<sup>x+</sup>/CeZrO<sub>2</sub>. Sequences of elementary steps are proposed and detailed kinetic rate laws were established. Simulations were performed using the global and the detailed rate equations. A good fitting was observed at low conversion. For high conversion, diffusion or thermodynamic limitations must be considered.

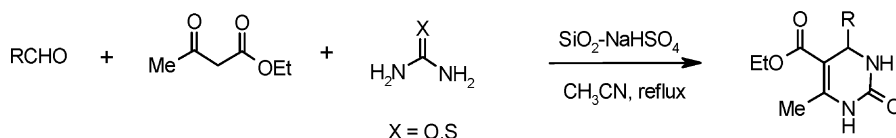


**M. Adharvana Chari, K. Syamasundar**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 137

Silicagel supported sodium hydrogensulfate as a heterogenous catalyst for high yield synthesis of 3,4-dihydropyrimidin-2 (1H)-ones

Silicagel supported sodium bisulfate catalyzes efficiently the three component condensation reaction of aldehyde, β-ketoester and urea in refluxing acetonitrile to afford the corresponding dihydropyrimidones. Compared to the classical Biginelli reaction conditions, this new approach consistently has the advantage of excellent yields (84–93%) and short reaction times 1–2.5 h.

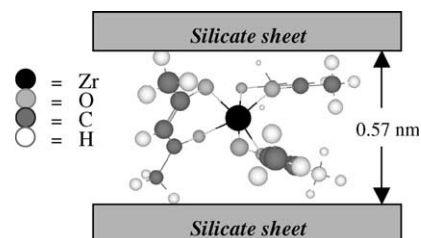


**Yessi Permana, Shogo Shimazu, Nobuyuki Ichikuni, Takayoshi Uematsu**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 141

Selective synthesis of primary methoxypropanol using clay supported tris(2,4-pentanedionato)zirconium(IV)

Primary methoxypropanol has been selectively synthesized from propylene oxide and methanol using clay supported tris(2,4-pentanedionato)zirconium(IV) catalyst, which was prepared by facile ion-exchange method. The immobilized zirconium complex demonstrated considerable increase in catalytic activity when it was employed in ring-opening reaction of propylene oxide and significant increase in selectivity compared to its homogeneous state.

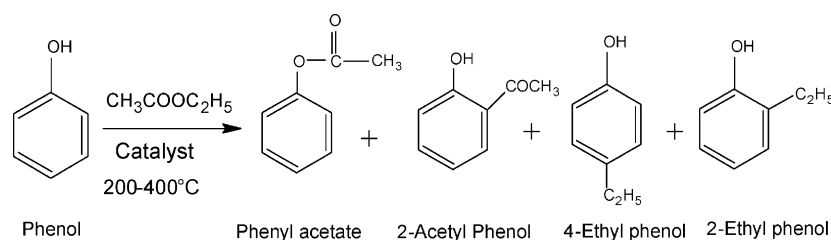


**K. Shanmugapriya, R. Anuradha, M. Palanichamy, Banumathi Arabindoo, V. Murugesan**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 145

Vapour phase reaction of phenol with ethyl acetate over MCM-41 molecular sieves

The vapour phase reaction of phenol with ethyl acetate was investigated over Al and Zn incorporated MCM-41 molecular sieves. Among the catalysts studied, Al-MCM-41(55) was more active than the other catalysts. At the optimal feed ratio (1:3) and WHSV (1.79 h<sup>-1</sup>) phenol conversion over Al-MCM-41(55) was 85.5% with high selectivity to 2-EP (63.3%).

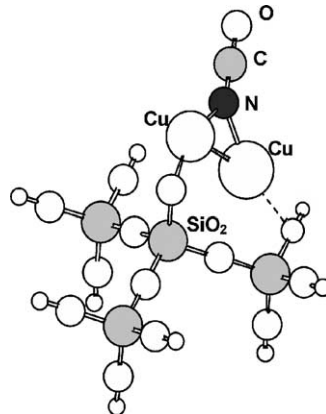


**Ricardo M. Ferullo, Norberto J. Castellani**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 155

NCO adsorption over SiO<sub>2</sub> and Cu/SiO<sub>2</sub> cluster models from density functional theory

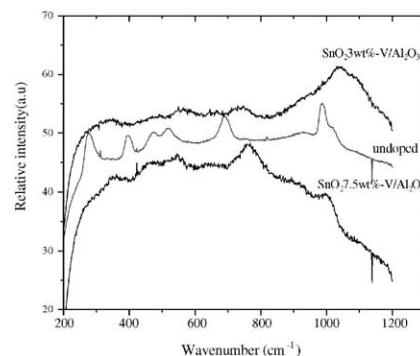
The adsorption of NCO over atomic and dimer copper deposited on silica defects were studied. While in the first case the support does not affect the Cu–NCO bonding, it enhances that interaction in the second case. This behaviour is related to the higher charge transfer from the dimer to NCO, which produces a strong Cu–NCO bonding which has an important ionic character.

**Yinghuan Fu, Hongchao Ma, Zhenlü Wang, Wanchun Zhu, Tonghao Wu, Guo-jia Wang**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 163

Characterization and reactivity of SnO<sub>2</sub>-doped V<sub>2</sub>O<sub>5</sub>/γ-Al<sub>2</sub>O<sub>3</sub> catalysts in dehydrogenation of isobutane to isobutene

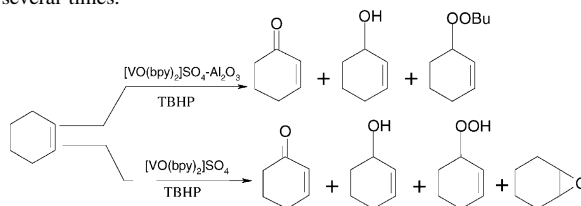
Raman spectra shows that Raman band of crystalline vanadia at 144, 199, 283, 405, 490, 524, 696 and 995 cm<sup>-1</sup> is not detected and Raman band of isolated monomeric vanadyl species at 1039 cm<sup>-1</sup> is observed after addition of tin. However, higher amounts of SnO<sub>2</sub> (7.5 wt.%) lead to the formation of more agglomerated vanadia (Raman band at 750 and 1006 cm<sup>-1</sup>).

**M. Salavati-Niasari, M.R. Elzami, M.R. Mansournia, S. Hydarzadeh**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 169

Alumina-supported vanadyl complexes as catalysts for the CH bond activation of cyclohexene with *tert*-butylhydroperoxide

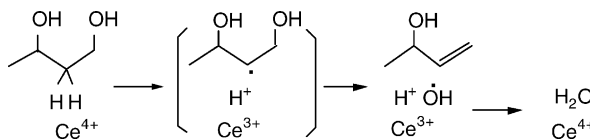
We synthesized several VO<sup>2+</sup> complexes of various ligands (en, TMED, bpy, phen, acac, salen, salophen) supported on acidic alumina. These solids were characterized by elemental analysis, IR and DRS spectroscopy and then used as catalysts in cyclohexene oxidation reaction by TBHP. The major products of the reaction were 2-cyclohexene-1-ol and 2-cyclohexene-1-one. [VO(bpy)<sub>2</sub>](SO<sub>4</sub>)Al<sub>2</sub>O<sub>3</sub> shows significantly higher catalytic activity than other alumina-supported complexes. Alumina-supported vanadyl catalysts with the nitrogen donor ligands show significantly higher catalytic activity than oxygen donor ligands at the same surface coverage. These catalysts can also be reused in the oxidation of cyclohexene for several times.

**Satoshi Sato, Ryoji Takahashi, Toshiaki Sodesawa, Nozomi Honda**

*Journal of Molecular Catalysis A: Chemical* 221 (2004) 177

Dehydration of diols catalyzed by CeO<sub>2</sub>

Dehydration of several 1,3-diols into unsaturated alcohols was investigated over pure CeO<sub>2</sub>. In the dehydration of 1,3-propanediol, 1,3-butanediol, 3-methyl-1,3-butanediol, 2,4-pentanediol, and 2-methyl-2,4-pentanediol, unsaturated alcohols are selectively produced at 325 °C.

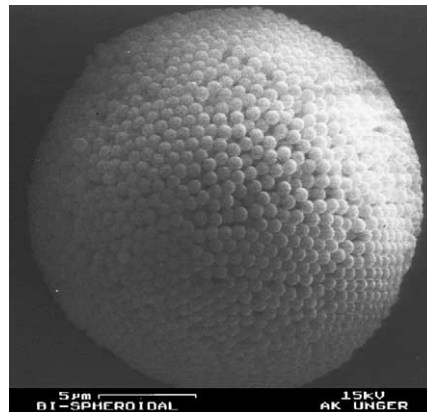


**Cedric du Fresne von Hohenesche,  
Klaus K. Unger, Thomas Eberle**

*Journal of Molecular Catalysis A: Chemical* 221  
(2004) 185

Agglomerated non-porous silica nanoparticles as  
model carriers in polyethylene synthesis

Spherical agglomerates were obtained by spray  
drying of non-porous submicron silica particles.  
The silica agglomerates were employed as model  
carriers in the heterogeneous polymerization of  
ethylene using a conventional methylaluminoxane  
(MAO)/ $\eta^5$ -dicyclopentadienyl zirconiumdichlor-  
ide metallocene catalyst system. The polymeriza-  
tion process depended more on the geometrical  
and structural aspects of the beads rather than on  
their specific surface areas.

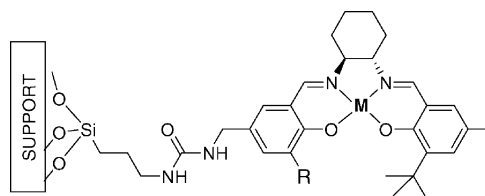


**V. Ayala, A. Corma, M. Iglesias, F. Sánchez**

*Journal of Molecular Catalysis A: Chemical* 221  
(2004) 201

Mesoporous MCM41-heterogenised (salen)Mn  
and Cu complexes as effective catalysts for oxida-  
tion of sulfides to sulfoxides. Isolation of a stable  
supported Mn(V)=O complex, responsible of the  
catalytic activity

Chiral salen manganese and copper complexes immobilised on mesoporous silica supports have been  
investigated as catalysts in the sulfide to sulfoxide oxidation. The presence of stable manganyl  
[Mn(V)=O] complexes into support channels have been established, being responsible for catalytic  
activity. The recovery and reusability of heterogenised Mn- and Cu-catalysts have been studied.



**A.I. Kryukov, A.L. Stroyuk, N.N. Zin'chuk,  
A.V. Korzhak, S.Ya. Kuchmii**

*Journal of Molecular Catalysis A: Chemical* 221  
(2004) 209

Optical and catalytic properties of Ag<sub>2</sub>S nanopar-  
ticles

Optical properties and catalytic activity of Ag<sub>2</sub>S  
nanoparticles in methylviologen and Ag<sup>+</sup> reduc-  
tion were investigated. It was shown that catalytic  
Ag<sup>+</sup> reduction can be accelerated at the irradiation  
of Ag<sub>2</sub>S colloids.

