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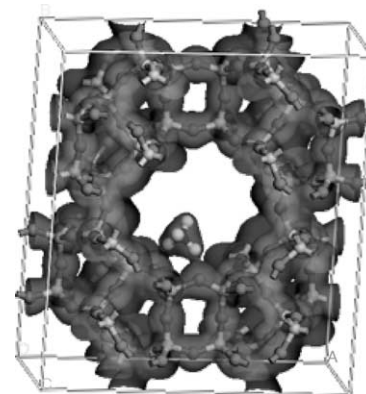
Articles

**M. Elanany, D.P. Vercauteren, M. Koyama,
M. Kubo, P. Selvam, E. Broclawik, A. Miyamoto**

*Journal of Molecular Catalysis A: Chemical 243
(2006) 1*

H-MOR: Density functional investigation for the relative strength of Brønsted acid sites and dynamics simulation of NH₃ protonation–deprotonation

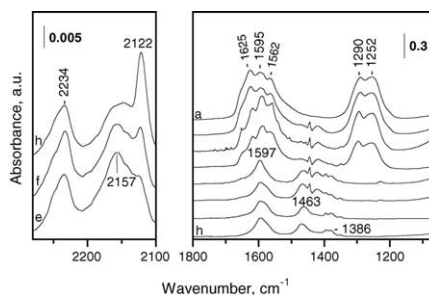
The adsorption energies of NH₃ on Brønsted acid sites in the main channel, side pocket, and double four-membered rings of H-MOR are investigated using DFT employing periodic models. Results reveal that E_{ads} on Brønsted acid sites in the main channel (T₄, T₂, and T₁) are higher than that in the side pocket (T3).



**Tzvetomir Venkov, Momchil Dimitrov,
Konstantin Hadjiivanov**

*Journal of Molecular Catalysis A: Chemical 243
(2006) 8*

FTIR spectroscopic study of the nature and reactivity of NO_x compounds formed on Cu/Al₂O₃ after coadsorption of NO and O₂

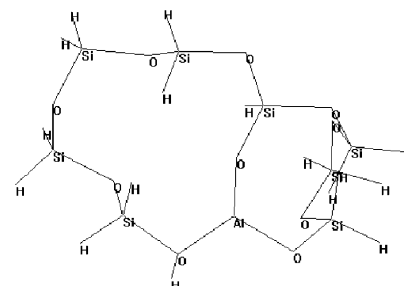


R. Dimitrova, G. Gündüz, M. Spassova

*Journal of Molecular Catalysis A: Chemical 243
(2006) 17*

A comparative study on the structural and catalytic properties of zeolites type ZSM-5, mordenite, Beta and MCM-41

Zeolites of different structures and textural mesoporosity (ZSM-5, mordenite, Beta and MCM-41) were studied. Zeolite framework irregularity, mesoporosity and acid sites dispersion had a major influence on the reactions as alpha-pinene isomerization and methanol conversion. Acidify is the governing factor for alpha-pinene isomerization in comparison with samples mesoporosity.

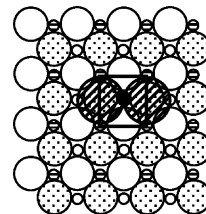


Haiyang Zhu, Yong Wu, Xi Zhao, Haiqin Wan, Lijuan Yang, Jianming Hong, Qing Yu, Lin Dong, Yi Chen, Can Jian, Jun Wei, Penghui Xu

Journal of Molecular Catalysis A: Chemical 243 (2006) 24

Influence of impregnation times on the dispersion of CuO on anatase

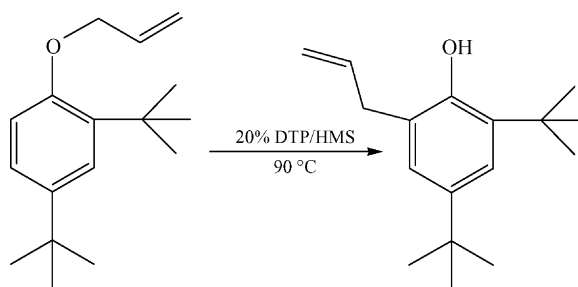
The dispersion capacity of copper oxide in CuO/TiO₂ samples with one-step impregnation and double-step impregnation are about 0.52 and 0.98 mmol/100 m² TiO₂, respectively, which should be related to the shielding effect of accompanying NO₃⁻ anions during the impregnations.



Ganapati D. Yadav, Sharad V. Lande

Journal of Molecular Catalysis A: Chemical 243 (2006) 31

Selective Claisen rearrangement of allyl-2,4-di-*tert*-butylphenyl ether to 6-allyl-2,4-di-*tert*-butylphenol catalysed by heteropolyacid supported on hexagonal mesoporous silica



Alexandre Rossi, Wagner F. De Giovanni

Journal of Molecular Catalysis A: Chemical 243 (2006) 40

Redox and spectral properties of [Ru(4,4'-Me₂bpy)₂(AsPh₃)(H₂O)](ClO₄)₂. Application to electrocatalytic oxidations of organic compounds

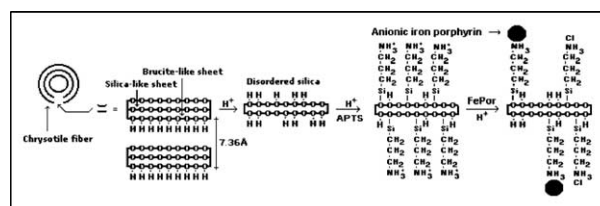
The complex [Ru(4,4'-Me₂bpy)₂(AsPh₃)(H₂O)](ClO₄)₂ (4,4'-Me₂bpy = 4,4'-dimethyl-2,2'-bipyridine) has been prepared and its spectral and redox properties have been investigated. The oxocomplex which is generated electrochemically from the aqua complex [(4,4'-Me₂bpy)₂(AsPh₃)Ru(H₂O)]²⁺ → [(4,4'-Me₂bpy)₂(AsPh₃)RuO]²⁺ + 2e + 2H⁺ has been used in homogeneous electrooxidations of benzyl alcohol, 1-phenylethanol and cyclohexene. The reactivity of this complex is compared to that of the analogous complex [Ru(4,4'-Me₂bpy)₂(PPh₃)(H₂O)](ClO₄)₂.

Matilte Halma, Alesandro Bail, Fernando Wypych, Shirley Nakagaki

Journal of Molecular Catalysis A: Chemical 243 (2006) 44

Catalytic activity of anionic iron(III) porphyrins immobilized on grafted disordered silica obtained from acidic leached chrysotile

Hydrated disordered silica obtained by leaching chrysotile with hydrochloric acid was grafted with 3-APTS and reacted with aqueous iron porphyrins solutions of [Fe(TDFSPP) and Fe(TCFSPP)]. The materials were characterized and investigated as catalysts in oxidation reaction of cyclohexane. The catalytic activities obtained in heterogeneous media for Fe(TDFSPP) was superior to the results obtained in homogeneous conditions but the opposite effect was observed for the Fe(TCFSPP), indicating that instead of the structural similarity of both iron porphyrins (second generation porphyrins), the immobilization way produced different catalysts.

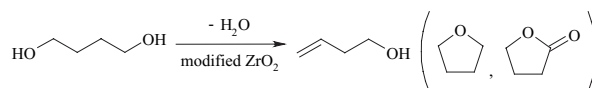


**Naoki Yamamoto, Satoshi Sato,
Ryoji Takahashi, Kanichiro Inui**

Journal of Molecular Catalysis A: Chemical 243
(2006) 52

Synthesis of 3-buten-1-ol from 1,4-butanediol over
ZrO₂ catalyst

1,4-Butanediol was selectively dehydrated into 3-buten-1-ol with producing a small amount of THF and γ -butyrolactone over sodium-modified ZrO₂ at temperatures of 325–375°C, where 3-buten-1-ol is possibly formed by acid–base bifunctional catalysis of monoclinic ZrO₂

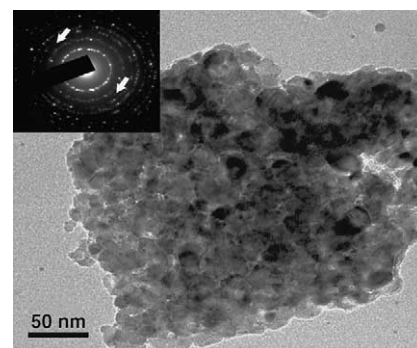


S. Rengaraj, X.Z. Li

Journal of Molecular Catalysis A: Chemical 243
(2006) 60

Enhanced photocatalytic activity of TiO₂ by doping
with Ag for degradation of 2,4,6-trichlorophenol in
aqueous suspension

A series of Ag-TiO₂ nanocatalysts were synthesized by doping with Ag onto TiO₂. The experimental results confirmed that the presence of Ag on TiO₂ catalysts could enhance the photocatalytic degradation of TCP in aqueous suspension significantly. A high extent of TCP mineralization was also achieved, in which while total organic carbon was reduced by 80% within 120 min, most chlorine on TCP was more quickly converted to chloride within the first 40 min.

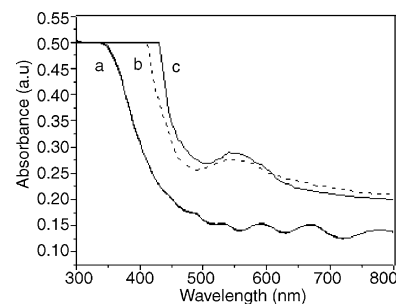


R.S. Sonawane, M.K. Dongare

Journal of Molecular Catalysis A: Chemical 243
(2006) 68

Sol-gel synthesis of Au/TiO₂ thin films for photo-
catalytic degradation of phenol in sunlight

The addition of colloidal Au in TiO₂ shifts absorption edge of TiO₂ films from 360 nm in UV to 430–440 nm in visible region. This increased absorption results in the 2–2.3 times enhancement in photo-catalytic activity of Au/TiO₂ thin film catalyst than undoped TiO₂ films.

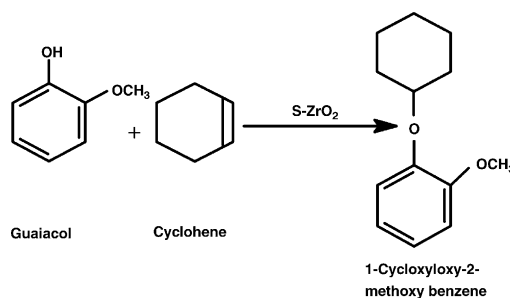


Ganapati D. Yadav, Ganesh S. Patre

Journal of Molecular Catalysis A: Chemical 243
(2006) 77

Chemoselective catalysis by sulphated zirconia in
O-alkylation of guaiacol with cyclohexene

Sulphated zirconia is used to promote etherification of guaiacol with cyclohexene very effectively.

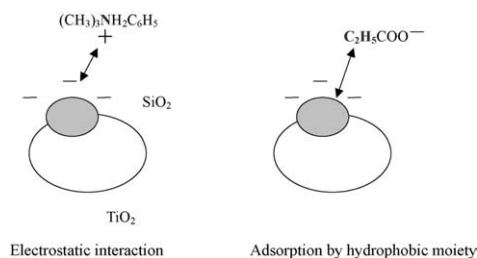


Y. Arai, K. Tanaka, A.L. Khlaifat

Journal of Molecular Catalysis A: Chemical 243 (2006) 85

Photocatalysis of SiO₂-loaded TiO₂

SiO₂-loading enhanced the photocatalytic activity of TiO₂ for the degradation of several substrates. The highest efficiency was observed for cationic compound, which was attributed to electrostatic interaction of negatively charged SiO₂/TiO₂ and cation. On the other hand simple mixing of SiO₂ with TiO₂ resulted in no effect.

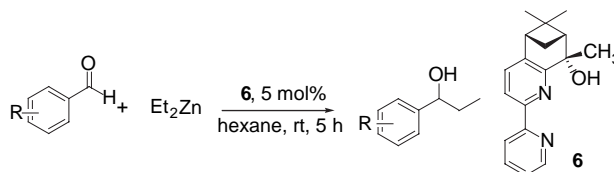
**Rong-Xin Lin, Chinpiao Chen**

Journal of Molecular Catalysis A: Chemical 243 (2006) 89

Chiral 8-substituted 10,10-dimethyl-5-pyridin-2-yl-6-aza-tricyclo[7.1.1.0^{2,7}]undeca-2(7),3,5-trien-8-ols as enantioselective catalysts in the addition of diethylzinc to substituted benzaldehydes

Chiral 8-substituted 10,10-dimethyl-5-pyridin-2-yl-6-aza-tricyclo[7.1.1.0^{2,7}]undeca-2(7),3,5-trien-8-ols as enantioselective catalysts in the addition of diethylzinc to substituted benzaldehydes.

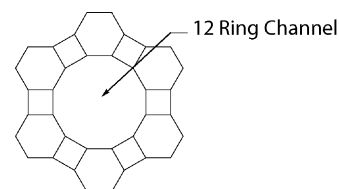
The derivatives of ligand **6** were prepared and assessed in the enantioselective addition of diethylzinc to substituted benzaldehydes providing the alcohols of (*S*)-configuration with enantiomeric excess generally ranging from 45 to 79%.

**K. Joseph Antony Raj, E.J. Padma Malar, V.R. Vijayaraghavan**

Journal of Molecular Catalysis A: Chemical 243 (2006) 99

Shape-selective reactions with AEL and AFI type molecular sieves alkylation of benzene, toluene and ethylbenzene with ethanol, 2-propanol, methanol and *t*-butanol

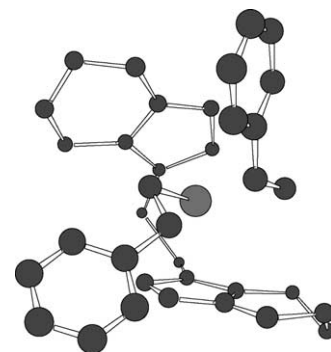
The vapour and liquid phase alkylation of various reactions are studied over MnAPO-5 and MnAPO-11. The product distribution and selectivity are discussed in terms of dimensions of the molecules. The studies suggest that a strong deactivation of the catalyst occurs with increase in bulkiness of the reactants. The vapour phase reactions carried out at high temperatures (350 and 400 °C) result in faster deactivation of the catalyst, whereas the liquid phase reactions showed good conversion and extended catalyst life.

**Nunzia Galdi, Carmela Della Monica, Aldo Spinella, Leone Oliva**

Journal of Molecular Catalysis A: Chemical 243 (2006) 106

Enantioselective C–C bond formation in styrene dimerization with chiral ansa zirconocene-based catalyst

The mixture of styrene and H₂ in the presence of the chiral ansa zirconocene (*R,R*)-ethylenebis tetrahydroindenyl zirconium dichloride and methylalumoxane affords optically active (*R*)-1,3-diphenylbutane (1,3-dpb). This product can be functionalized without loss of chirality, e.g. to 2-methylglutaric acid. The study on the complex regiochemical behavior of this hydroooligomerization catalysis allowed the optimization of the 1,3-dpb yield and suggests the possible improvement of the catalyst performance.



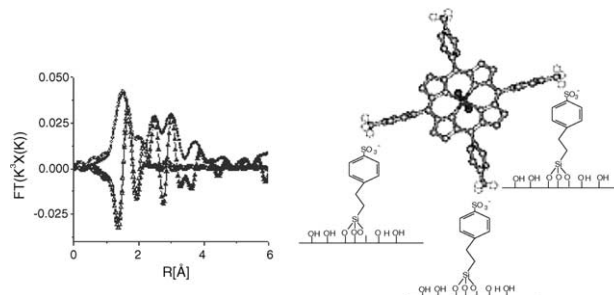
**Alba D.Q. Ferreira, Fábio S. Vinhado,
Y. Iamamoto**

Journal of Molecular Catalysis A: Chemical 243
(2006) 111

Characterization of Mn(III)porphyrin immobilized on modified silica surfaces by EXAFS spectroscopy: A promising tool for analysis of supported metalloporphyrin catalysts

The first Mn–K edge EXAFS spectra recorded for catalytic materials containing manganese(III)porphyrin $[\text{Mn}\{\text{T}(4\text{-}N\text{-MePy})\text{P}\}(\text{L})_2]^{5+}$ ($\text{L} = \text{oxygenated}$ or nitrogenated ligands)-grafted onto functionalized

silica surfaces, which have been used in hydrocarbon oxygenations, gave structural evidences about the coordination environment of the active sites and their interaction nature with the silica matrix.



William W. Yu, Hanfan Liu

Journal of Molecular Catalysis A: Chemical 243
(2006) 120

Singular modification effects of metal cations and metal complex ions on the catalytic properties of metal colloidal nanocatalysts

Adsorbed metal cations motivates the polar C=O group, then the nearby dissociated H atoms attack the C and O atoms of C=O group to generate a hydroxyl group. This electron transfer from nanocatalyst to the adsorbed metal cation boosts the adsorbing ability of C=O double bond onto the nanocatalyst surface, therefore increases the activity and the selectivity of nanocatalysts.

