

## Contents

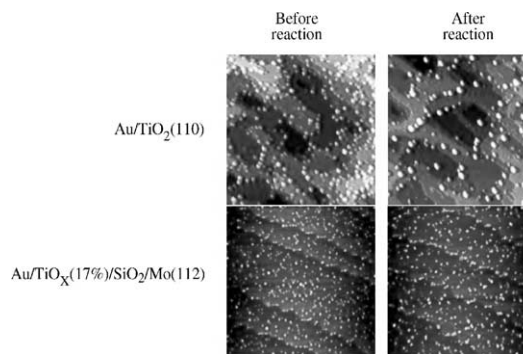
### Articles

**W.T. Wallace, B.K. Min, D.W. Goodman**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 3

The stabilization of supported gold clusters by surface defects

Gold clusters supported on titania and silica substrates ( $\text{Au}/\text{TiO}_2$  and  $\text{Au}/\text{SiO}_2$ ) sinter when exposed to high temperatures and reaction pressures. By synthesizing a mixed titania-silica thin film possessing small  $\text{TiO}_x$  islands, the sintering of gold clusters can be inhibited.

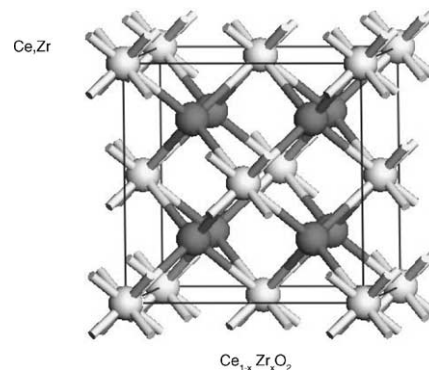


**J.A. Rodriguez, X. Wang, G. Liu, J.C. Hanson, J. Hrbek, C.H.F. Peden, A. Iglesias-Juez, M. Fernández-García**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 11

Physical and chemical properties of  $\text{Ce}_{1-x}\text{Zr}_x\text{O}_2$  nanoparticles and  $\text{Ce}_{1-x}\text{Zr}_x\text{O}_2(111)$  surfaces: synchrotron-based studies

Synchrotron-based techniques (high-resolution photoemission, time-resolved X-ray diffraction (XRD), and X-ray absorption near-edge spectroscopy) were used to investigate the physical and chemical properties of  $\text{Ce}_{1-x}\text{Zr}_x\text{O}_2$  nanoparticles and  $\text{Ce}_{1-x}\text{Zr}_x\text{O}_2(111)$  surfaces ( $x \leq 0.5$ ).

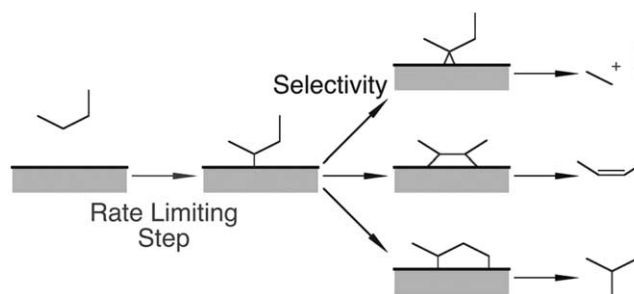


**Francisco Zaera**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 21

Tuning selectivity in hydrocarbon conversion catalysis

In catalysis, the rate-limiting step (the initial C–H bond activation in alkanes) may be different than those responsible for defining selectivity ( $\alpha$ -,  $\beta$ -, or  $\gamma$ -hydride elimination reactions).

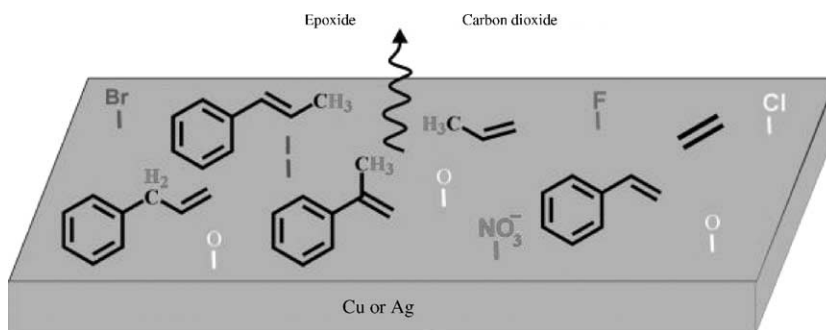


**Richard M. Lambert, Federico J. Williams,  
Rachael L. Cropley, Alejandra Palermo**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 27

Heterogeneous alkene epoxidation: past, present  
and future

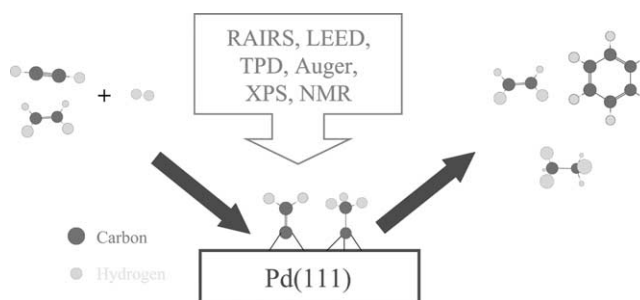
Ag and Cu-catalysed heterogeneous epoxidation of alkenes is a strong function of the identity of the metal, the presence or otherwise of allylic H atoms, and the stereochemistry of the alkene. Halogens and nitrate promote selectivity by an electronic effect and direct oxygen transfer, respectively.



**D. Stacchiola, F. Calaza, T. Zheng,  
Wilfred T. Tysoe**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 35

Hydrocarbon conversion on palladium catalysts

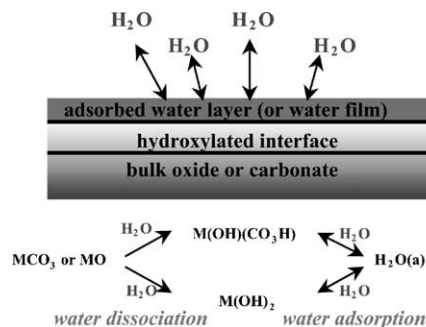


**Hind A. Al-Abadleh, Hashim A. Al-Hosney,  
Vicki H. Grassian**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 47

Oxide and carbonate surfaces as environmental  
interfaces: the importance of water in surface  
composition and surface reactivity

Under environmental conditions, water changes the composition of oxide and carbonate surfaces from that of the bulk. Hydroxyl groups and adsorbed water play important roles in the chemistry of these interfaces.



**Brian E. Hayden, Michael E. Rendall,  
Oliver South**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 55

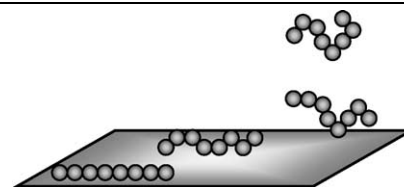
The stability and electro-oxidation of carbon  
monoxide on model electrocatalysts: Pt(111)-  
Sn(2x2) and Pt(111)-Sn( $\sqrt{3} \times \sqrt{3}$ )R30°

**Andrew J. Gellman, Kris R. Paserba,  
Nithya Vaidyanathan**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 67

A comparative study of the kinetics and energetics  
of oligomer desorption from graphite

Conformational isomerism of adsorbed oligo-  
meric species such as long chain alkanes or poly-  
ethylene glycols has been shown to impact their  
desorption kinetics.

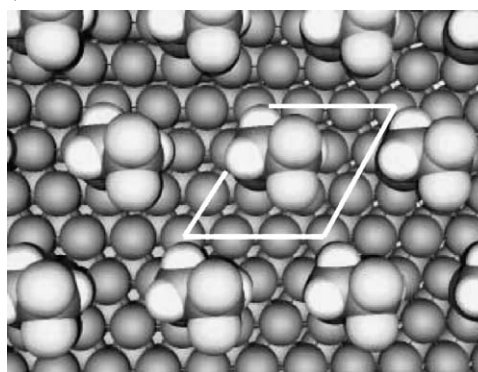


**Xin Li, Andrew J. Gellman, David S. Sholl**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 77

Orientation of ethoxy, mono-, di-, and tri-fluoro  
ethoxy on Cu(111): a DFT study

Density functional theory has been used to determine the orientation of ethoxy, mono-, di-, and tri-fluoroethoxy on Cu(111).

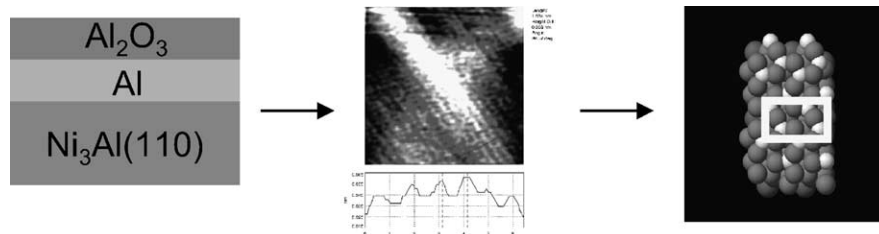


**F. Qin, N.P. Magtoto, J.A. Kelber, D.R. Jennison**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 83

Theory and experiments on the structure of 7Å  
alumina films grown on Ni<sub>3</sub>Al

STM shows that 7Å thick well-ordered Al<sub>2</sub>O<sub>3</sub>/Ni<sub>3</sub>Al(110) films are Kappa-like alumina, in agreement with DFT calculations. The calculations also predict the presence of internal voids which may store atomic hydrogen.



**L.A. Avalos, V. Bustos, R. Uñac, F. Zaera,  
G. Zgrablich**

*Journal of Molecular Catalysis A: Chemical* 228  
(2005) 89

Toward a realistic model for the kinetics of the  
NO+CO reaction on rhodium surfaces

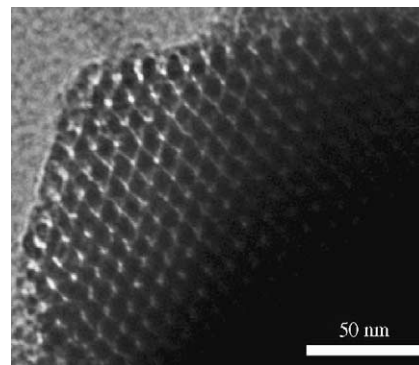
A model for the kinetics of NO reduction by CO on  
Rh(111) surfaces is proposed that takes into  
account the formation of N-islands in the adsorbed  
phase, an increase of the NO dissociation proba-  
bility with the number of neighboring vacant  
sites, and the blocking of NO dissociation due  
to the presence of neighboring coadsorbed NO and  
CO species. The effect and importance of each  
elementary process in the reaction kinetics is  
discussed.

**J.M. Esparza, M.L. Ojeda, A. Campero, G. Hernández, C. Felipe, M. Asozoa, S. Cordero, I. Kornhauser, F. Rojas**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 97

Development and sorption characterization of some model mesoporous and microporous silica adsorbents

Mesoporous and microporous silica substrates were prepared via sol-gel and micelle templating and characterized through N<sub>2</sub> sorption. Materials consisting of: cage-like cavities interconnected by narrow throats (SBA-16), individual cylindrical pores of about the same size (SBA-15), sinuous ganglion-like sequences of bulges and throats (mesoporous glass), and nanoparticle arrangements (microporous SiO<sub>2</sub>) were studied by remarking their outstanding morphological and sorption qualities.

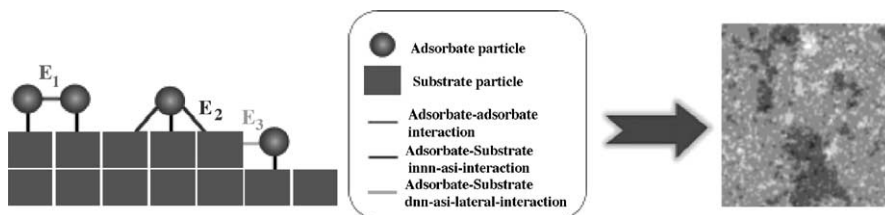


**C. De Micco, S.E. Guidoni, D.A. Mirabella, C.M. Aldao**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 111

Surface roughening due to adsorbates

We show how adsorbates can induce surface roughening. Monte Carlo simulations were used to explore adsorbate-adsorbate repulsion and adsorbate-substrate interactions that lead to changes in the surface morphology.

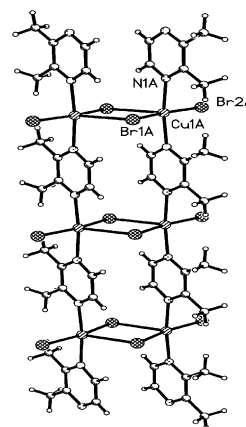


**Brian M. Wells, Christopher P. Landee, Mark M. Turnbull, Firas F. Awwadi, Brendan Twamley**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 117

Design and synthesis of magnetic ladders: structure and magnetic properties of Cu(2,3-dimethylpyrazine)Br<sub>2</sub>

The title compound has been prepared and its crystal structure and magnetic properties determined. The compound crystallizes as a coordination polymer and forms a ladder structure. Magnetic susceptibility data support the magnetic ladder structure for the material

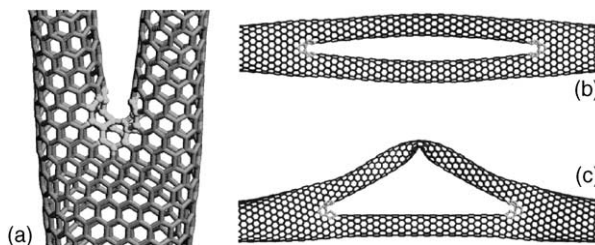


**A. Latgé, D. Grimm, P. Venezuela**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 125

Y-shaped carbon nanotubes: structural stability and transport properties

A topological defect, composed of six heptagons, induces the bifurcation of a main carbon nanotube into two smaller ones, forming a Y-structure. Three examples of equilibrium atomic configurations are shown: a Y-junction (a) and two kinds of YJ-rings, called as symmetric (b) and asymmetric (c), depending upon the equivalence between the lengths of the two arms composing the ring, respectively. We study the dependence of the energy formation and total energy with temperature for the Y-ring structures. A polymerization process for the case of symmetric ring is predicted.

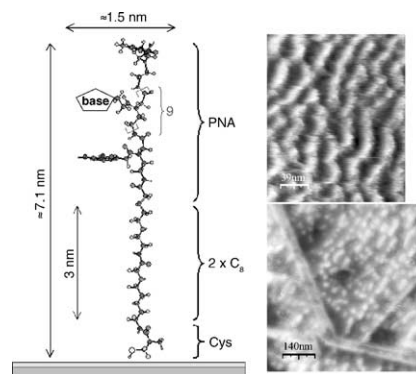


**C. Briones, E. Mateo-Martí,  
C. Gómez-Navarro, V. Parro, E. Román,  
J.A. Martín-Gago**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 131

Structural and functional characterization of self-assembled monolayers of peptide nucleic acids and its interaction with complementary DNA

Ordered self-assembled monolayers (SAMs) of single-stranded peptide nucleic acid (ssPNA) molecules can be formed on gold surfaces, with efficient capability for recognizing complementary ssDNA. By X-ray photoemission spectroscopy and atomic force microscopy, we proved that in spite of their remarkable length (6–7nm), ssPNA molecules can assemble standing-up on the surface similar to the SAMs of short alkanethiols.



**George G. Kleiman**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 137

Electronic structure information of metals and alloys from auger and photoemission

We report electronic structure changes in AuZn, AuMg, AuPd, AgPd and CuNi from XPS and Auger shifts. Charge transfer in AuPd, CuPd, AgPd, AuCu, AgAu and CuNi seems negligible.

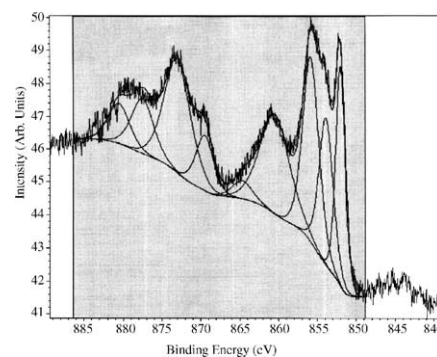
XPS + Auger Spectra $\Rightarrow$	Energy Shifts $\Rightarrow$	Charge Transfer + $d$ and $sp$ changes
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**Pedro A.P. Nascente**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 145

Materials characterization by X-ray photoelectron spectroscopy

X-ray photoelectron spectroscopy (XPS) is one of the most used surface analysis techniques for the characterization of materials, including those used as catalysts.

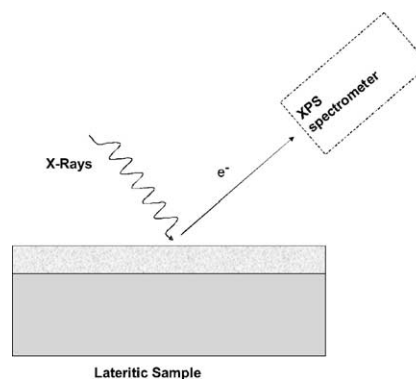


**J. Mendialdua, R. Casanova, F. Rueda,  
A. Rodríguez, J. Quiñones, L. Alarcón,  
E. Escalante, P. Hoffmann, I. Taebi,  
L. Jalowiecki**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 151

X-ray photoelectron spectroscopy studies of laterite standard reference material

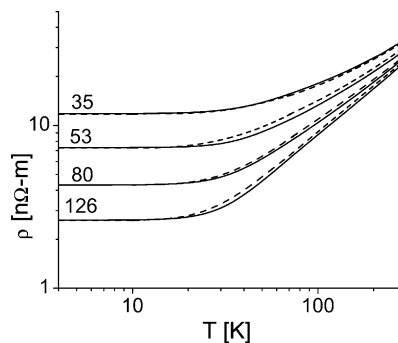
The characterization of two lateritic natural samples (certified geologically) by XPS shows the presence of some kind of iron aluminate on their surface.



**Raul C. Munoz**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 163

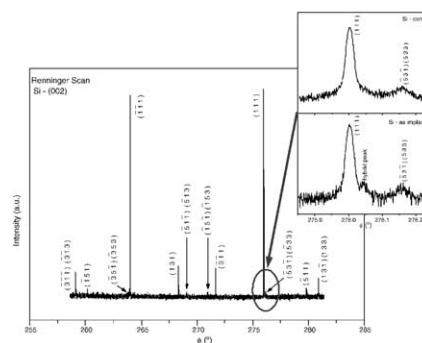
Resistivity induced by a rough surface of thin gold films deposited on mica

**R.V. Orloski, M.A.A. Pudenzi, M.A. Hayashi, J.W. Swart, L.P. Cardoso**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 177

X-ray multiple diffraction on the shallow junction of B in Si(001)

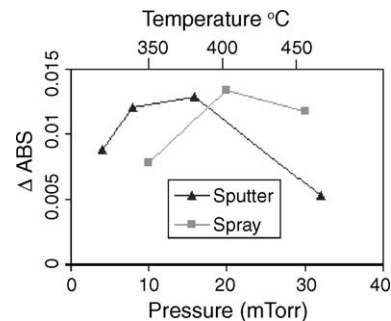
The hybrid extra Bragg surface diffraction (BSD) peak representing the contribution from the interstitial rich region in the matrix Renninger scan (RS), was used as a fine interface probe to investigate this region as a function of the implantation energy and the thermal annealing condition. The possibility of applying this structural characterization technique to other systems (such as single crystal model catalysts) is intriguing.

**Dwight R. Acosta, Arturo I. Martínez, Alcidez A. López, Carlos R. Magaña**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 183

Titanium dioxide thin films: the effect of the preparation method in their photocatalytic properties

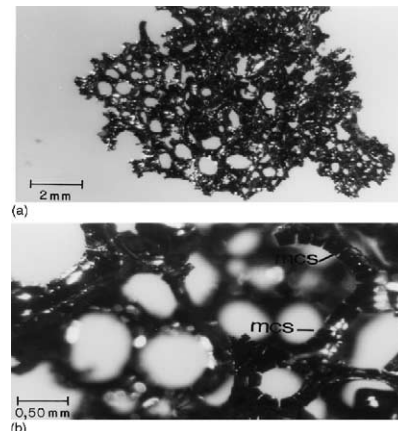
The behavior of photodegradation of methylene blue on  $\text{TiO}_2$  thin films when illuminated with UV radiation can be observed in the graphic. For films deposited by magnetron sputtering the variation is followed for pressure increasing in the sputtering chamber. For films deposited by spray pyrolysis the influence of substrate temperature on the photocatalytic activity of  $\text{TiO}_2$  thin films can be followed from the graphic. The best results are obtained in films deposited at 16mTorr and with  $T_s=400^\circ\text{C}$ , respectively.

**J. Matos, M. Labady, A. Albornoz, J. Laine, J.L. Brito**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 189

Catalytic effect of KOH on textural changes of carbon macro-networks by physical activation

The synthesis and definition of the topological organization of polygonal macro-networks of carbon have been performed by a two-step controlled pyrolysis of saccharose. From the study of textural changes of three-dimensional samples, a detailed mechanism that involves the role of KOH as a catalyst for the activation of the macro-networks has been proposed.

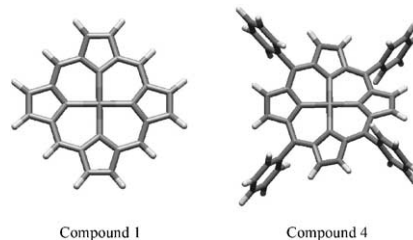


**Isidoro García-Cruz, José Manuel Martínez-Magadán, Fernando Alvarez-Ramírez, Roberto Salcedo, Francesc Illas**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 195

Theoretical study of nickel porphyrinate derivatives related to catalyst dopant in the oil industry

Ni-porphyrinate is totally planar hence exhibiting a marked difference with respect to the analogous vanadyl compound which has been shown to have a dome shape. The Ni-porphyrinates studied in the present work exhibit a slight non-planar shape. The origin of this strain has been attributed to the reduced space of the porphyrin molecule cavity and also to the presence of peripheral substituents. It appears that the largest deviation from planarity occurs in the case of phenyl substituents whereas in both aliphatic cases a similar strain is predicted. This feature could be attributed to a large increase in the electronic density near the metal center caused by the presence of the aromatic rings.

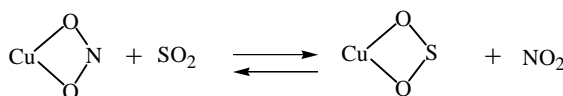


**Anibal Sierraalta, Aleida Bermudez, Marcos Rosa-Brussin**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 203

Density functional study of the interaction of Cu<sup>+</sup> ion-exchanged zeolites with H<sub>2</sub>O and SO<sub>2</sub> molecules

DFT calculations were carried out to study the interaction of H<sub>2</sub>O, SO<sub>2</sub>, O<sub>2</sub>, NO<sub>2</sub> and NO with a model of Cu-zeolite. The results indicate a chemical equilibrium between the NO<sub>x</sub> and the adsorbed H<sub>2</sub>O. The SO<sub>2</sub> binds stronger to Cu than O<sub>2</sub> and similar to H<sub>2</sub>O. The Bader's analysis show the activation of the O<sub>2</sub> and SO<sub>2</sub> molecules by Cu.

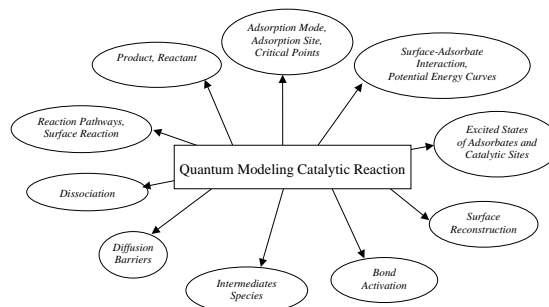


**Fernando Ruetter, Morella Sánchez, Anibal Sierraalta, Claudio Mendoza, Rafael Añez, Luis Rodríguez, Orlando Lisboa, Judith Daza, Pastor Manrique, Zhandra Perdomo, Marcos Rosa-Brussin**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 211

Application of computational methods to catalytic systems

In this work we analyze the complexity of: catalytic processes considering different areas of chemistry, physics, and engineering; quantum catalytic modeling; surface processes; and energy flux at the reaction center. A survey of the most recent and relevant computational modeling work using ab initio methods is made as well as some applications to the parametric method CATIVIC.

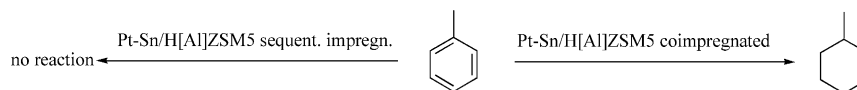


**Ricardo Morales, Luis Melo, Aura Llanos, Francisco Zaera**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 227

Characterization of bifunctional PtSn/H[Al]ZSM5 catalysts: a comparison between two impregnation strategies

The type of impregnation strategy used to prepare PtSn/H[Al]ZSM5 catalysts lead to pronounced changes in the catalytic behavior because of the presence of an electronic effect between Pt and Sn for the co-impregnated samples and a geometric effect for the sequentially impregnated samples. All samples were characterized by using the toluene hydrogenation reaction, X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy.





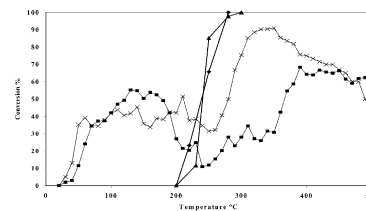


**Grisel Corro, J.L.G. Fierro, Ramón Montiel, Fortino Bañuelos**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 275

Improved sulfur resistance of Pt-Sn/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalysts for C<sub>3</sub>H<sub>8</sub>-NO-O<sub>2</sub> reaction under lean conditions due to Pt-Sn surface interactions

The selective catalytic reduction (SCR) of NO with C<sub>3</sub>H<sub>8</sub> was studied over unsulfated and pre-sulfated 1% Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, and 1% Pt-2% Sn/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalysts. Carbon residues deposited were evaluated on all samples, after 12h of C<sub>3</sub>H<sub>8</sub>-NO-O<sub>2</sub>-SO<sub>2</sub> reaction. Pre-sulfated 1% Pt-2% Sn/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst showed a high resistance on deactivation by sulfur and on carbon residues deposition. Results are explained on basis of X-ray photoelectron spectra (XPS) showing that tin addition to 1% Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> resulted in (i) lowering the sulfates generated over the surface of the catalyst; (ii) preventing Pt particles from sintering during sulfation process; and (iii) decrease in the number of sites available on the alumina for carbon residues species to be adsorbed.

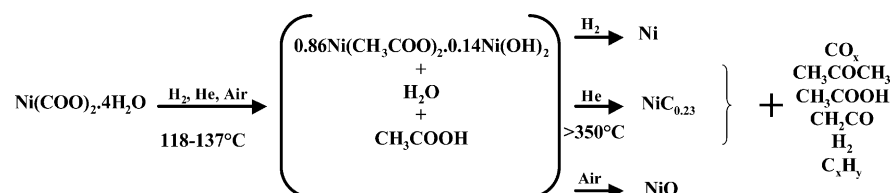


Effect of temperature on the C<sub>3</sub>H<sub>8</sub>-NO-O<sub>2</sub>-SO<sub>2</sub> reaction over pre-sulfated 1% Pt/Al<sub>2</sub>O<sub>3</sub>: (○) C<sub>3</sub>H<sub>8</sub>; (■) NO; and pre-sulfated 1% Pt-2% Sn/Al<sub>2</sub>O<sub>3</sub>: (▲) C<sub>3</sub>H<sub>8</sub>; (◆) NO. Feed: 1000 ppm of NO, 2.5 vol % C<sub>3</sub>H<sub>8</sub>, 50 ppm of SO<sub>2</sub>, 15 vol % of O<sub>2</sub>, and balance He.

**Juan C. De Jesus, Ismael González, Angel Quevedo, Tito Puerta**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 283

Thermal decomposition of nickel acetate tetrahydrate: an integrated study by TGA, QMS and XPS techniques

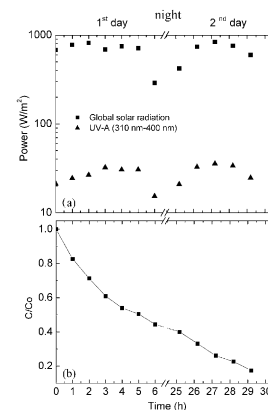


**Edward Carpio, Patricia Zúñiga, Silvia Ponce, José Solís, Juan Rodríguez, Walter Estrada**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 293

Photocatalytic degradation of phenol using TiO<sub>2</sub> nanocrystals supported on activated carbon

Titanium oxide supported on activated carbon pellet could complete phenol degradation in a continuous irradiation during different days. It is also observed that in between the irradiation times, the adsorption of phenol continue but in a low quantity.



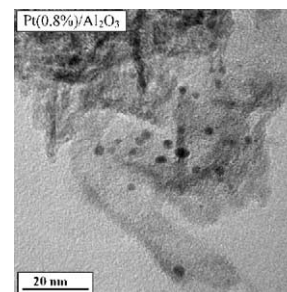
**J.M. Ramallo-López, F.G. Requejo, A.F. Craievich, J. Wei, M. Avalos-Borja, E. Iglesia**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 299

Complementary methods for cluster size distribution measurements: supported platinum nanoclusters in methane reforming catalysts

Pt cluster size strongly influences the reactivity of surfaces for C-H bond activation during CH<sub>4</sub> steam reforming. C-H bond activation turnover rates for H<sub>2</sub>O reforming of CH<sub>4</sub> increased with decreasing Pt cluster size, suggesting that coordinatively unsaturated surface Pt atoms are more reactive than Pt atoms in low-index surfaces prevalent in larger clusters. Near-edge fine structure in X-ray absorption spectra clearly shows electronic changes in Pt clusters relative to bulk Pt crystallites, though differences in the 5d electronic density among samples with different cluster size could not be related directly to Pt surface atom coordination. These results suggest that catalytic consequences of cluster size arise from surface structure changes leading to coordinative unsaturation of surface atoms.

X-ray absorption and small angle X-ray scattering techniques were used to measure the size of Pt metal nanoclusters and the results are compared with H<sub>2</sub> chemisorption and transmission electron microscopy data.

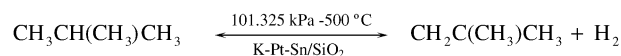


**D. Rodríguez, J. Sánchez, G. Arteaga**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 309

Effect of tin and potassium addition on the nature of platinum supported on silica

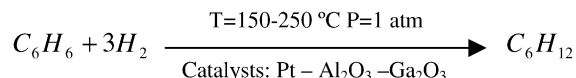
This study aimed to examine the effects of tin and potassium addition on the catalytic properties of Pt/SiO<sub>2</sub>. Temperature programmed reduction (TPR), UV-vis spectroscopy by diffuse reflectance (DRS) and CO chemisorption were used to characterize these catalysts. The activity of the catalyst was determined by the isobutane dehydrogenation

**Francisco Domínguez, Jorge Sánchez, Geomar Arteaga, Eduardo Choren**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 319

Gallia as support of Pt in benzene hydrogenation reaction

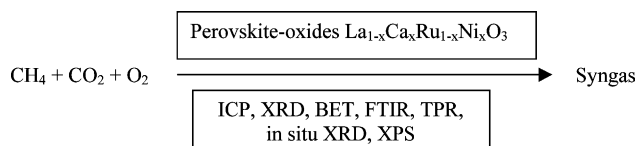
The aim of this work was to study the effect of gallia on the catalytic behavior for hydrogenation reactions of platinum supported on alumina. Gallia/alumina supported Pt catalysts were prepared. The catalysts were characterized by X-ray diffraction, nitrogen adsorption, temperature-programmed reduction (TPR), carbon monoxide chemisorption and thermogravimetric analysis. The benzene hydrogenation reaction was used to test the catalytic activity.

**M.R. Goldwasser, M.E. Rivas, E. Pietri, M.J. Pérez-Zurita, M.L. Cubeiro, A. Grivobal-Constant, G. Leclercq**

*Journal of Molecular Catalysis A: Chemical* 228 (2005) 325

Perovskites as catalysts precursors: synthesis and characterization

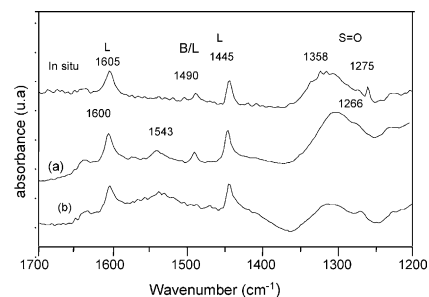
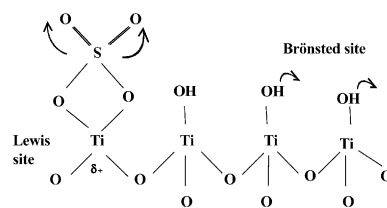
Perovskites type oxides La<sub>1-x</sub>Ca<sub>x</sub>Ru<sub>1-x</sub>Ni<sub>x</sub>O<sub>3</sub> catalysts were developed to transform CH<sub>4</sub> and CO<sub>2</sub>, two cheap contaminating chemicals, to more valuable feedstock such as syngas. Characterization was performed to obtain a better appreciation of the principles underlying the modification of metal catalysts by promoters by total or partial substitution of A- and B-site cations. The influence of Ru partial substitution by Ni in the LaRuO<sub>3</sub> structure and of La by Ca on LaRu<sub>0.8</sub>Ni<sub>0.2</sub>O<sub>3</sub> was also investigated in the dry and combine reforming of methane. After reduction Ru(Ni) crystallites size in the order of 10–15nm were produced. Correlation between the effect of partial or total substitution of La by Ca as A-site cation of the precursor perovskite on the catalytic activity and stability of in situ formed Ru(Ni) particles was established.

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Catalytic behavior of sulfated TiO<sub>2</sub> in light olefins oligomerization

Isobutene oligomerization over sulfated TiO<sub>2</sub>, prepared by three methods was investigated: (i) “in situ” sulfation using sulfuric acid, (ii) gelling with nitric acid and sulfation (a) and (iii) gelling with ammonium hydroxide and sulfation (b). The samples showed L/B ratios of 3.65, 1.82 and 1.25, respectively. It is proposed that, for the butenes oligomerization on sulfated TiO<sub>2</sub>, at higher L/B ratio catalyst stability is improved.

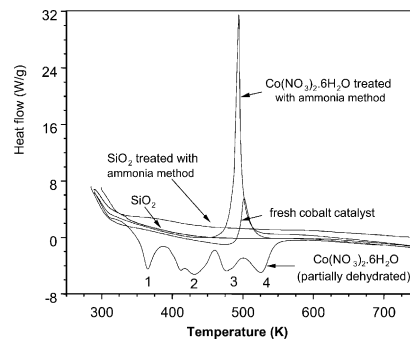


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Heavier alcohols synthesis on cobalt phyllosilicate catalysts

Differential scanning calorimetry studies on cobalt catalysts synthesized with the ammonia method and its precursors, indicated the formation of cobalt aqua-complex that interact with the silica aerosil 200 forming Co-phyllsilicate.



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High selectivity to isopropyl ether over sulfated titania in the isopropanol decomposition

It was found that in sulfate  $\text{TiO}_2$  prepared from titanium alkoxide and gelled with sulfuric acid, the super acid sites centers must be Lewis acid sites associated to the metal cation. Acid strength is strongly enhanced by an electron induction effect of  $\text{S}=\text{O}$  as shown in the scheme.

