



## Contents

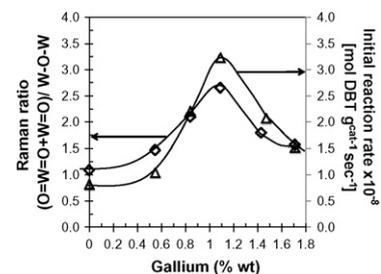
### Articles

**J.N. Díaz de León, M. Picquart, M. Villarroel,  
M. Vrinat, F.J. Gil Llambias, F. Murrieta,  
J.A. de los Reyes**

*Journal of Molecular Catalysis A: Chemical 323 (2010) 1*

Effect of gallium as an additive in hydrodesulfurization  
WS<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> catalysts

Raman spectroscopy showed that gallium incorporation had a strong effect in the formation of WO<sub>x</sub> species at the surface of catalysts. Our results confirm clearly a positive effect of Ga on the HDS activity for WS<sub>2</sub> catalysts.

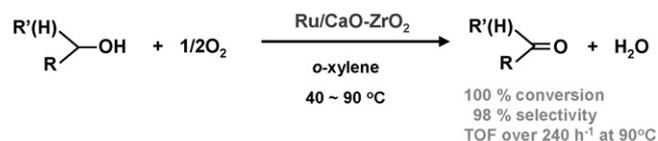


**Takashi Yasu-eda, Susumu Kitamura,  
Na-oki Ikenaga, Takanori Miyake,  
Toshimitsu Suzuki**

*Journal of Molecular Catalysis A: Chemical 323 (2010) 7*

Selective oxidation of alcohols with molecular oxygen over Ru/CaO–ZrO<sub>2</sub> catalyst

Aerobic oxidation of alcohols was successfully carried out by the RuCl<sub>3</sub> loaded on CaO–ZrO<sub>2</sub> basic solid solution supported catalyst.

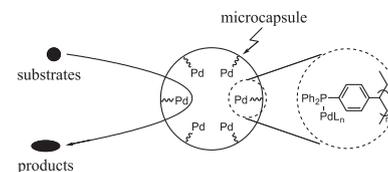


**Ying Liu, Xiujuan Feng, Decai Bao, Kaixiao Li,  
Ming Bao**

*Journal of Molecular Catalysis A: Chemical 323 (2010) 16*

A new method for the preparation of microcapsule-supported palladium catalyst for Suzuki coupling reaction

Highly monodispersed microcapsules containing phosphine ligand were synthesized and palladium was then attached to the interior of the microcapsules. These microcapsules acted as microreactors in which the catalysis occurred.

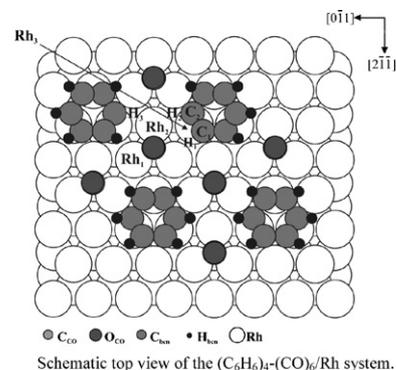


**Paula V. Jasen, Estela A. González,  
Graciela Brizuela, Alfredo Juan**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 23

A bonding study of CO–benzene co-adsorption on Rh(1 1 1)

The co-adsorption of carbon monoxide and benzene on Rh(1 1 1) has been studied using density functional calculations. We used the ordered  $p(3 \times 30)$  surface unit cell. The hydrogen of the benzene ring presents a bonding angle of  $26^\circ$ . The CO–benzene interaction is very weak and a small  $H_{\text{benzene}-\text{C}_{\text{CO}}}$  OP of 0.001 is detected. The Rh–Rh overlap population decreases 36.7% after co-adsorption.

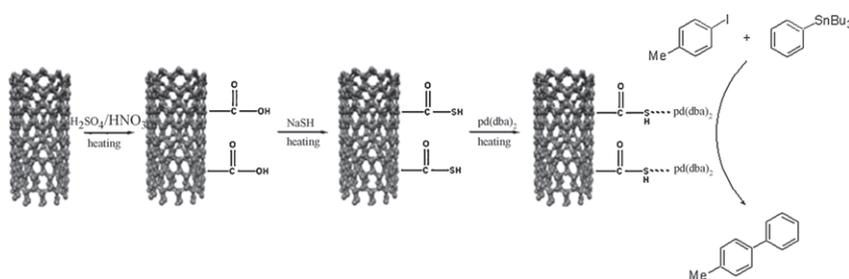


**Ja Young Kim, Youngshin Jo, Seong-Keun Kook,  
Sunwoo Lee, Hyun Chul Choi**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 28

Synthesis of carbon nanotube supported Pd catalysts and evaluation of their catalytic properties for C–C bond forming reactions

A simple method of depositing Pd nanoparticles onto carbon nanotubes (CNTs) as catalyst supports is devised for C–C bond forming reactions. A high-yield CC bond forming reaction accomplished at a low Pd content and in the absence of any ligand is observed.

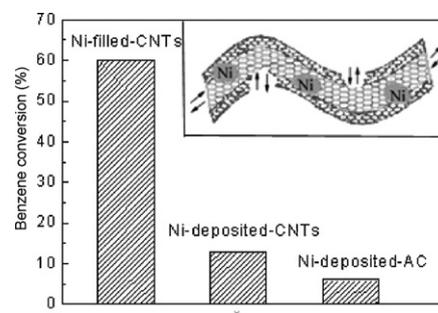


**Hongxiao Yang, Shaoqing Song, Richuan Rao,  
Xizhang Wang, Qing Yu, Aimin Zhang**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 33

Enhanced catalytic activity of benzene hydrogenation over nickel confined in carbon nanotubes

The dramatic increase of the catalytic activity over the Ni confined in the inner of multi-walled carbon nanotubes with more defects has been interpreted by the facile reduction, reinforced reactivity, increased reactants density, and larger gaps formed on sidewall of carbon nanotubes which could reduce the diffusion resistance kinetically.

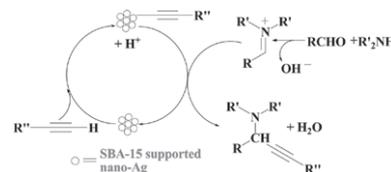


**Guo-Ping Yong, Dong Tian, Hong-Wu Tong,  
Shao-Min Liu**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 40

Mesoporous SBA-15 supported silver nanoparticles as environmentally friendly catalysts for three-component reaction of aldehydes, alkynes and amines with glycol as a “green” solvent

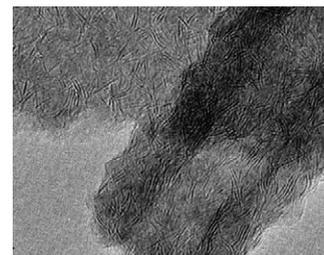
Mesoporous SBA-15 supported silver nanoparticles can catalyze  $A^3$ -coupling reaction of aldehydes, alkynes and amines in more environmentally friendly medium with glycol as “green” solvent. The catalysts could be recovered easily and used repetitively four times. It is also found that the maximum reaction yield has been obtained for an average Ag-nanoparticle size of about 8 nm.



Z.D. Huang, W. Bensch, A. Lotnyk, L. Kienle,  
S. Fuentes, J. Bocarando, G. Alonso, C. Ornelas

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 45

SBA-15 as support for NiMo HDS catalysts derived from sulfur-containing molybdenum and nickel complexes: Effect of activation mode

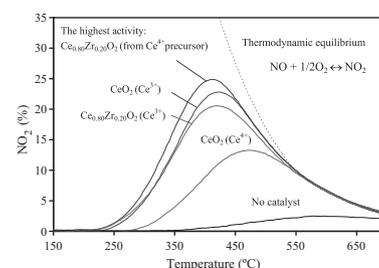


Noelia Guillén-Hurtado, Idriss Atribak,  
Agustín Bueno-López, Avelina García-García

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 52

Influence of the cerium precursor on the physico-chemical features and NO to NO<sub>2</sub> oxidation activity of ceria and ceria-zirconia catalysts

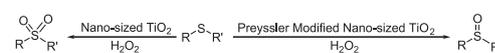
The preparation of Ce<sub>0.80</sub>Zr<sub>0.20</sub>O<sub>2</sub> mixed oxides was conducted by coprecipitation, using either Ce(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O or (NH<sub>4</sub>)<sub>2</sub>Ce(NO<sub>3</sub>)<sub>6</sub>, as cerium precursor. The samples were characterised by N<sub>2</sub> adsorption at -196 °C, XRD, Raman spectroscopy, XRF, H<sub>2</sub>-TPR and XPS and the structural differences found as well as their NO to NO<sub>2</sub> oxidation capacities were discussed.



Mohammad Rahimizadeh, Ghadir Rajabzadeh,  
Seyed-Mola Khatami, Hossein Eshghi, Ali Shiri

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 59

TiO<sub>2</sub> nanoparticles and Preyssler-type heteropoly acid modified nano-sized TiO<sub>2</sub>: A facile and efficient catalyst for the selective oxidation of sulfides to sulfones and sulfoxides

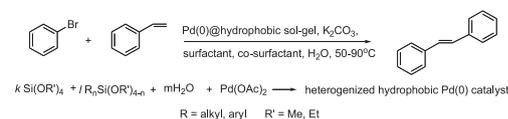


Alina Rozin-Ben Baruch, Dmitry Tselikhovsky,  
Michael Schwarze, Reinhard Schomäcker,  
Monzer Fanun, Jochanan Blum

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 65

Dependence of the Heck coupling in aqueous microemulsion by supported palladium acetate on the surfactant and on the hydrophobicity of the support

Heck coupling of bromobenzene and styrene in water by sol-gel entrapped palladium acetate depends on the hydrophobicity of the ceramic support and on the electronic nature of the surfactant.

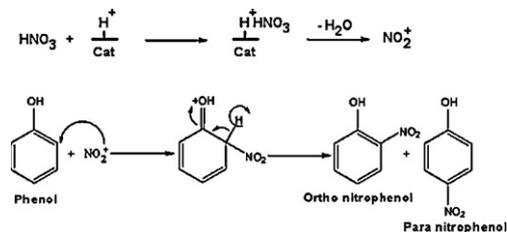


**S.M. Kemdeo, V.S. Sapkal, G.N. Chaudhari**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 70

TiO<sub>2</sub>-SiO<sub>2</sub> mixed oxide supported MoO<sub>3</sub> catalyst: Physicochemical characterization and activities in nitration of phenol

Reaction proceeds via formation of nitronium ions over the Brönsted acid sites of the catalyst and later attack of those at ortho- and para-position of phenol.

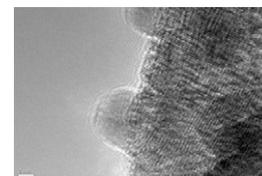


**M.A. Gondal, A. Bagabas, A. Dastageer, A. Khalil**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 78

Synthesis, characterization, and antimicrobial application of nano-palladium-doped nano-WO<sub>3</sub>

The loading of nano-palladium on *n*-WO<sub>3</sub> enhanced the photo-catalytic activity of *n*-WO<sub>3</sub> for the removal of *Escherichia coli* microorganism from water under 355-nm UV laser irradiation.

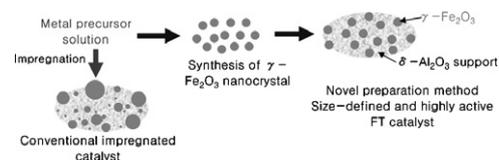


**Jo-Yong Park, Yun-Jo Lee, Pawan K. Khanna, Ki-Won Jun, Jong Wook Bae, Young Ho Kim**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 84

Alumina-supported iron oxide nanoparticles as Fischer-Tropsch catalysts: Effect of particle size of iron oxide

Homogeneously sized iron oxide nanocrystals of 2.0–12.0 nm were prepared and supported on alumina to evaluate a crystal size effect on Fischer-Tropsch reaction.



**Zhiqiang Zhang, Yixin Qu, Shui Wang, Jidong Wang**

*Journal of Molecular Catalysis A: Chemical* 323 (2010) 91

Theoretical study on the mechanisms of the conversion of methyl lactate over sodium polyphosphate catalyst

Quantum chemical calculations indicate that decomposition of methyl lactate to acrylic acid and methanol and decarbonylation of methyl lactate to acetaldehyde, methanol and CO are the predominant pathways over sodium tripolyphosphate, a model of NaH<sub>2</sub>PO<sub>4</sub>/SiO<sub>2</sub> catalyst.

