



## Contents

### Articles

**Arumugam Murugadoss, Hidehiro Sakurai**

*Journal of Molecular Catalysis A: Chemical 341 (2011) 1*

Chitosan-stabilized gold, gold–palladium, and gold–platinum nanoclusters as efficient catalysts for aerobic oxidation of alcohols

► New preparative methods for the chitosan stabilized metal nanoclusters. ► The produced NCS were uniform in size distribution ( $2.3 \pm 0.2$  nm). ► Efficient catalytic activity toward the aerobic oxidation of various alcohols. ► Comparable catalytic activity to previously reported Au:PVP catalysts. ► Heterogeneous catalysts and can be reused several times.

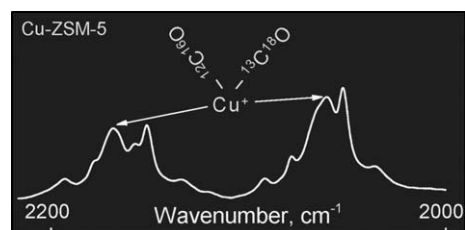


**Nicola Drenchev, Peter A. Georgiev, Konstantin Hadjiivanov**

*Journal of Molecular Catalysis A: Chemical 341 (2011) 7*

FTIR study of  $^{12}\text{C}^{16}\text{O}$  and  $^{13}\text{C}^{18}\text{O}$  coadsorption on Cu–ZSM-5

►  $^{12}\text{C}^{16}\text{O}$ – $^{13}\text{C}^{18}\text{O}$  isotopic mixtures are useful for establishing of polycarbonyl structures. ► Two kinds of  $\text{Cu}^+(\text{CO})_2$  species are formed on Cu–ZSM-5. ► Bands of tricarbonyls with one or two  $^{13}\text{C}^{18}\text{O}$  ligands are determined.

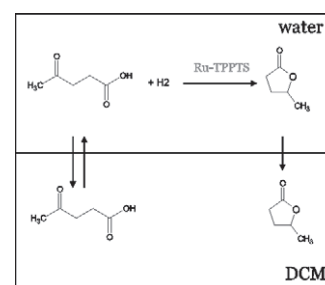


**M. Chalid, A.A. Broekhuis, H.J. Heeres**

*Journal of Molecular Catalysis A: Chemical 341 (2011) 14*

Experimental and kinetic modeling studies on the biphasic hydrogenation of levulinic acid to  $\gamma$ -valerolactone using a homogeneous water-soluble Ru–(TPPTS) catalyst

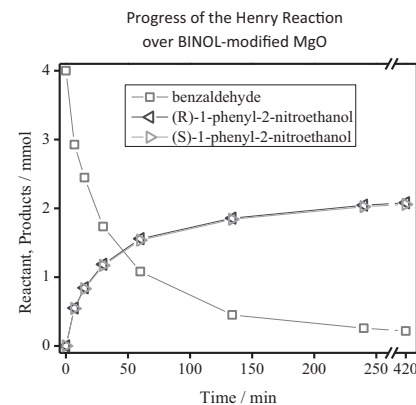
► Biphasic catalysis was applied to hydrogenate levulinic acid to  $\gamma$ -valerolactone. ► Quantitative GVL yields were obtained with a water soluble Ru–TPPTS catalyst. ► The experimental data were successfully quantified with a kinetic model. ► Recycling of the homogeneous catalyst was successfully demonstrated.



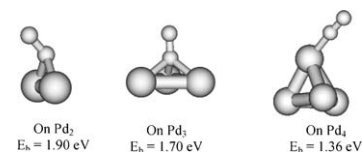
**Yuanzhou Xi, Robert J. Davis***Journal of Molecular Catalysis A: Chemical* 341 (2011) 22

Nanocrystalline MgO catalysts for the Henry reaction of benzaldehyde and nitromethane

► Nano-MgO is an effective catalyst for reaction of benzaldehyde and nitromethane. ► The areal rate on MgO is not affected by thermal treatment between 523 and 823 K. ► No enantiomeric excess is observed in products formed over S-BINOL-modified MgO.

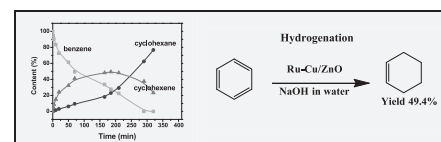
**C. Lacaze-Dufaure, J. Roques, C. Mijoule, E. Sicilia, N. Russo, V. Alexiev, T. Mineva***Journal of Molecular Catalysis A: Chemical* 341 (2011) 28A DFT study of the NO adsorption on Pd<sub>n</sub> (n = 1–4) clusters

► DFT study of the adsorption process of the NO molecule on small palladium clusters (n = 1–4). ► Full optimization of the NOPd<sub>n</sub> species. ► N–O binding energy strongly weakened by adsorption on Pd<sub>n</sub>. ► Dissociation process of NO on Pd<sub>4</sub> cluster highly improbable.

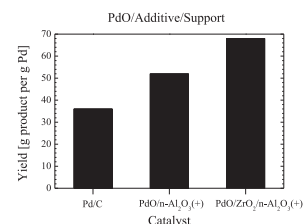
**Huizhen Liu, Shuguang Liang, Weitao Wang, Tao Jiang, Buxing Han***Journal of Molecular Catalysis A: Chemical* 341 (2011) 35

The partial hydrogenation of benzene to cyclohexene over Ru–Cu catalyst supported on ZnO

► Catalysts for selective hydrogenation of benzene to cyclohexene. ► Ru–Cu/ZnO prepared by deposition-precipitation, impregnation and coprecipitation. ► Characterized by TEM, SEM, XRD, XPS and nitrogen adsorption-desorption. ► NaOH significantly improved selectivity when using deposition-precipitation method. ► A maximum yield of cyclohexene 49.4%.

**Justin J. Dodson, Luke M. Neal, Helena E. Hagelin-Weaver***Journal of Molecular Catalysis A: Chemical* 341 (2011) 42The influence of ZnO, CeO<sub>2</sub> and ZrO<sub>2</sub> on nanoparticle-oxide-supported palladium oxide catalysts for the oxidative coupling of 4-methylpyridine

► Complex interactions between PdO, added oxide and support oxide identified. ► Too strong PdO-additive oxide interactions → palladium leaching or coverage. ► ZnO not a promoter, CeO<sub>2</sub> → unstable catalysts (too strong interactions). ► ZrO<sub>2</sub> is a true promoter for Al<sub>2</sub>O<sub>3</sub>-supported catalysts. ► PdO/ZrO<sub>2</sub>/n-Al<sub>2</sub>O<sub>3</sub>(+) prepared via coprecipitation best catalyst to date.

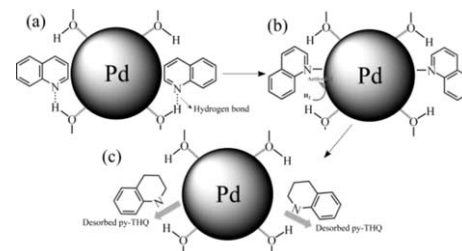


Hui Mao, Chen Chen, Xuepin Liao, Bi Shi

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 51

Catalytic hydrogenation of quinoline over recyclable palladium nanoparticles supported on tannin grafted collagen fibers

► Fibrous heterogeneous Pd catalyst. ► A highly stable and active heterogeneous Pd catalyst. ► Partial catalytic hydrogenation of quinoline. ► High activity, selectivity and reusability.

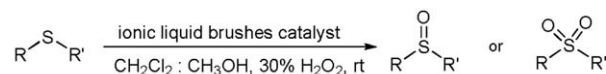


Xianying Shi, Xiaoyan Han, Wenjuan Ma, Junfa Wei, Jing Li, Qiang Zhang, Zhanguo Chen

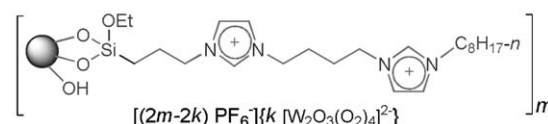
*Journal of Molecular Catalysis A: Chemical* 341 (2011) 57

Peroxo-tungstates immobilized on multilayer ionic liquid brushes-modified silica as an efficient and reusable catalyst for selective oxidation of sulfides with  $H_2O_2$

► Peroxo-tungstates held in different supported ionic liquid brushes catalysts were synthesized. ► The catalysts combine the advantages of ionic liquid, PTC and peroxy-tungstate catalyst together. ► The catalyst both exhibit high catalytic activities and provide excellent chemoselectivities. ► There was no apparent loss of catalyst efficiency until the 8th cycle. ► The use of  $H_2O_2$  as oxidant makes the reaction possess the advantages of green and clean.



ionic liquid brushes catalyst:

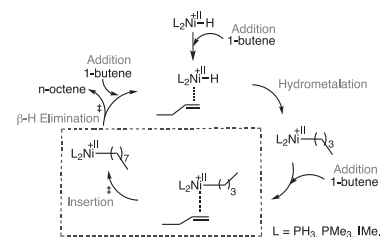


Ioannis Nikiforidis, Andreas Göring, Wolfgang Hieringer

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 63

On the regioselectivity of the insertion step in nickel complex catalyzed dimerization of butene: A density-functional study

► Mechanism of 1-butene dimerization investigated using density-functional theory. ► Nickel complex catalyst with phosphine or N-heterocyclic carbene ligands. ► Regioselectivity of olefin insertion in favor of low branching ratios. ► N-heterocyclic carbenes more active in insertion step than phosphines.

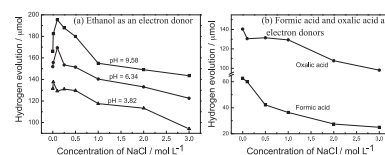


Yuexiang Li, Fang He, Shaoqin Peng, Dan Gao, Gongxuan Lu, Shuben Li

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 71

Effects of electrolyte NaCl on photocatalytic hydrogen evolution in the presence of electron donors over Pt/TiO<sub>2</sub>

► We investigate effect of NaCl on photocatalytic  $H_2$  evolution with electron donors. ► In ethanol system,  $Na^+$  adsorbed at photocatalyst  $TiO_2$  increases the  $H_2$  evolution. ► In formic acid or oxalic acid system, adsorbed  $Cl^-$  decreases the  $H_2$  evolution.

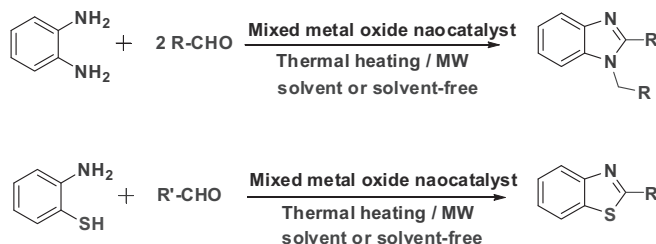


**Prabal Bandyopadhyay, Manisha Sathe,  
G.K. Prasad, Pratibha Sharma, M.P. Kaushik**

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 77

Mesoporous mixed metal oxide nanocrystals: Efficient and recyclable heterogeneous catalysts for the synthesis of 1,2-disubstituted benzimidazoles and 2-substituted benzothiazoles

► Synthesis of benzimidazoles and benzothiazoles using mixed metal oxide nanocatalyst. ► Catalyst characterization was performed by XRD, SEM and  $N_2$  BET analysis. ► High substrate/catalyst weight ratio, reusability are unique properties of catalyst. ► Catalyst with microwave heating was helpful in reducing time and increasing yields. ► Other features are cost-effective, clean reaction, simple work-up and high yields.

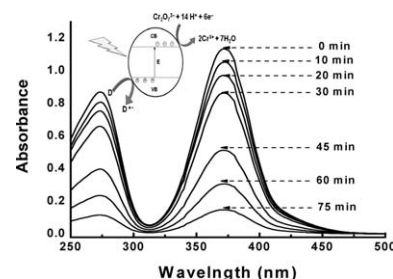


**M. Qamar, M.A. Gondal, Z.H. Yamani**

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 83

Synthesis of nanostructured NiO and its application in laser-induced photocatalytic reduction of Cr(VI) from water

► NiO nanoparticles using sol-gel method were synthesized and applied in photocatalytic reduction of Cr(VI) using a 355 nm laser radiation. ► Morphology of NiO nanoparticles was studied. ► ~90% Cr(VI) was removed within short laser exposure time. ► Effect of critical parameters was investigated.

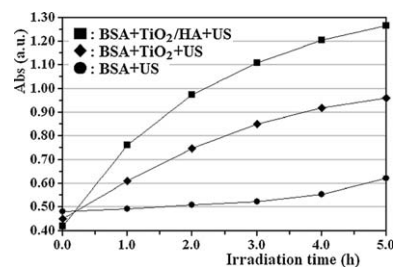


**Xudong Jin, Yuwei Guo, Jun Wang, Zhiqiu Wang,  
Jingqun Gao, Pingli Kang, Ying Li,  
Xiangdong Zhang**

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 89

The preparation of TiO<sub>2</sub>/hydroxylapatite (TiO<sub>2</sub>/HA) composite and sonocatalytic damage to bovine serum albumin (BSA) under ultrasonic irradiation

► Coating composite TiO<sub>2</sub>/hydroxylapatite (TiO<sub>2</sub>/HA) was prepared by precipitation method. ► TiO<sub>2</sub>/HA composite is used to study the sonodynamic damage to BSA molecules. ► Binding and damaging sites of TiO<sub>2</sub>/HA to BSA is studied by synchronous fluorescence technology. ► Some influence factors on the sonodynamic damage to BSA molecules were reviewed.



**Petr Štěpnička, Miloslav Semler, Jan Demel,  
Arnošt Zukal, Jiří Čejka**

*Journal of Molecular Catalysis A: Chemical* 341 (2011) 97

Reductive dehalogenation of aryl halides over palladium catalysts deposited on SBA-15 type molecular sieve modified with amine donor groups

► Pd catalysts deposited on SBA-15 type support modified with amine groups. ► Catalysts for reductive dehalogenation of haloarenes with formate as the H-source. ► Recyclable and efficient catalysts allowing for selective halogen removal.

