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# Journal of Catalysis

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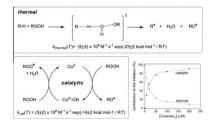
Journal of Catalysis Vol. 287, 2012

# **Contents**

### **PRIORITY COMMUNICATION**

# Thermal and catalytic formation of radicals during autoxidation

Ulrich Neuenschwander, Ive Hermans\*

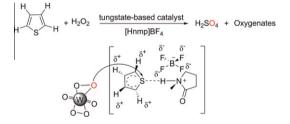


Quantitative insight was obtained in the formation of radicals during the autoxidation of the renewable olefin  $\alpha$ -pinene, decoupling thermal and catalytic contributions to the chain-initation.

### **REGULAR ARTICLES**

# Catalytic oxidation of thiophene and its derivatives via dual activation for ultra-deep desulfurization of fuels

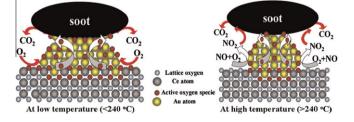
Boyu Zhang, Zongxuan Jiang, Jun Li, Yongna Zhang, Feng Lin, Yan Liu\*, Can Li\*



A catalytic system composed of ammonium tungstate and a Brønsted acidic ionic liquid (BAIL) [Hnmp]BF4 was found to be highly active for the oxidative removal of thiophene, benzothiophene, and their derivatives from model oil using 30 wt.% aqueous H<sub>2</sub>O<sub>2</sub> as the oxidant under mild condition.

### The catalysts of three-dimensionally ordered macroporous $Ce_{1-x}Zr_xO_2$ -supported gold nanoparticles for soot combustion: The metal-support interaction

Yuechang Wei, Jian Liu, Zhen Zhao\*, Aijun Duan, Guiyuan Jiang



The catalytic activities of 3DOM Au/Ce1-xZrx02 materials for soot oxidation are strongly related to the metal (Au)-supports (Ce) interaction. At low temperature, the soot particles are direct oxidized by active oxygen species migrated from the surface of supported Au catalysts. At high temperatures, the combined effects of active oxygen species and NO<sub>2</sub> enhance the rate of soot combustion.





pp 5-12

pp 1-4

pp 13-29

### Nanostructured MnO<sub>x</sub> as highly active catalyst for CO oxidation

Krisztina Frey\*, Viacheslav Iablokov, György Sáfrán, János Osán, István Sajó, Rafal Szukiewicz, Sergey Chenakin, Norbert Kruse\*

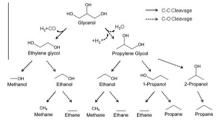
pp 30-36

Non-stoichiometric Mn-oxide ( $MnO_x$ ) with high specific surface area (525 m<sup>2</sup> g<sup>-1</sup>) shows high catalytic activity in CO oxidation reaction.

### **Correlation of Pt–Re surface properties with reaction pathways for the aqueous-phase reforming of glycerol** Liang Zhang, Ayman M. Karim, Mark H. Engelhard, Zhehao Wei, David L. King\*, Yong Wang\*

pp 37-43

pp 44-54



The major reaction pathways for aqueous-phase reforming of glycerol show the dependence of product selectivity on C–C bond cleavage (metal site-based) vs. C–O bond cleavage (acid site-based).

#### Effect of reduction in liquid phase on the properties and the catalytic activity of Pd/Al<sub>2</sub>O<sub>3</sub> catalysts

Elena Groppo\*, Giovanni Agostini, Andrea Piovano, Naresh B. Muddada, Giuseppe Leofanti, Riccardo Pellegrini, Giuseppe Portale, Alessandro Longo, Carlo Lamberti

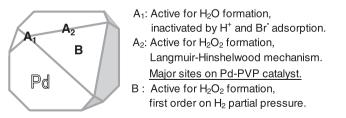
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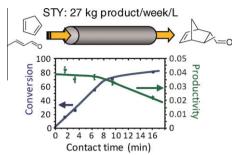
Relationships between the reduction state of a supported palladium catalyst, its surface structural properties, and its catalytic performance are investigated in a multi-technique approach.

**Dynamics of direct H<sub>2</sub>O<sub>2</sub> synthesis from H<sub>2</sub> and O<sub>2</sub> on a Pd nano-particle catalyst protected with polyvinylpyrrolidone pp 55–61 Takashi Deguchi, Hitoshi Yamano, Masakazu Iwamoto<sup>\*</sup>** 



Kinetics of the direct  $H_2O_2$  synthesis from  $H_2$  and  $O_2$  and  $Br^-$  adsorption behaviors on a Pd–PVP colloid catalyst in water containing  $H^+$  and  $Br^-$  ions was quite different from those on a Pd/C catalyst, which proposed improved classification of Pd surface sites active for the  $H_2O_2$  synthesis.

### Alumina-grafted macro-/mesoporous silica monoliths as continuous flow microreactors for the Diels–Alder reaction pp 62–67 A. Sachse, V. Hulea, A. Finiels, B. Coq, F. Fajula, A. Galarneau\*



Aluminum oxide-grafted silica monoliths were proved as highly productive catalytic microreactors for the in-flow implementation of the Diels-Alder reaction. Control of contact time and monolithic length has allowed to overcome external diffusion limitations.

# The effect of solvent addition on fructose dehydration to 5-hydroxymethylfurfural in biphasic system over zeolites pp 68–75

V.V. Ordomsky, J. van der Schaaf, J.C. Schouten, T.A. Nijhuis\*

Solvent addition significantly improved the selectivity to HMF in the aqueous phase dehydration of fructose over zeolite catalysts. The solvent not only improves the selectivity by extraction of the HMF produced, but also changes the intrinsic activity of the catalyst.

Time, min

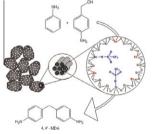
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Zeolite

# Efficient Sc triflate mesoporous-based catalysts for the synthesis of 4,4'-methylenedianiline from aniline and 4-aminobenzylalcohol

Selectivity to HN

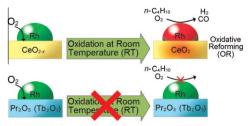
Natalia Candu, Madalina Ciobanu, Petru Filip, Jamal El Haskouri, Carmen Guillem, Pedro Amoros\*, Daniel Beltran, Simona M. Coman\*, Vasile I. Parvulescu\*



Isolated scandium triflate species incorporated in a UVM-7 porous bimodal support were prepared using a two-step strategy. These catalysts showed a high selectivity in the synthesis of 4, 40-methylenedianiline from aniline and 4-aminobenzylalcohol under mild conditions.

# Effect of the nature of rhodium catalyst supports on initiation of H<sub>2</sub> production during *n*-butane oxidative reforming pp 86–92 at room temperature

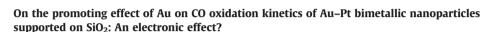
Katsutoshi Nagaoka\*, Katsutoshi Sato, Yusaku Takita



Oxidative reforming of *n*-butane was triggered rapidly at room temperature over  $Rh/CeO_{2-x}$  but not over  $Rh/Pr_2O_3$  and  $Rh/Tb_2O_3$ . The unique ability of  $CeO_{2-x}$  unlike  $Pr_2O_3$  and  $Tb_2O_3$ , to be oxidized at room temperature played a crucial role in triggering oxidative reforming at room temperature.

### Variation of residence time with chain length for products in a slurry-phase Fischer-Tropsch reactor

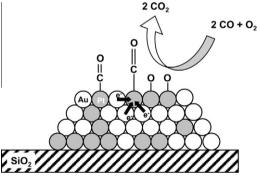
Cornelius Mduduzi Masuku\*, Wilson Davis Shafer, Wenping Ma, Muthu Kumaran Gnanamani, Gary Jacobs, Diane Hildebrandt, David Glasser, Burtron H. Davis



Residence time increase with carbon number up to  $C_{22}$ , the major removal method for products lighter than  $C_{10}$  is the gas phase while products between  $C_{10}$  and  $C_{22}$  are removed by both the vapor and the liquid flow.

Rachel P. Doherty, Jean-Marc Krafft, Christophe Méthivier, Sandra Casale, Hynd Remita, Catherine Louis, Cyril Thomas\*

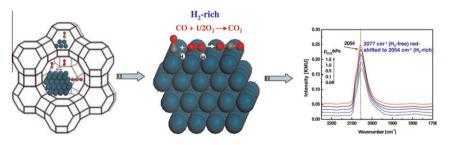
Products heavier than C<sub>22</sub> have the same residence time as the polywax.



A promoting effect of Au is reported on the kinetics of CO oxidation over Pt on AuPt bimetallic nanoparticles supported on SiO<sub>2</sub>. This is attributed to a greater electron density of the Pt surface atoms due to charge transfer from Au to Pt, as indicated by XPS and CO-FTIR.

#### Mechanistic study of preferential CO oxidation on a Pt/NaY zeolite catalyst

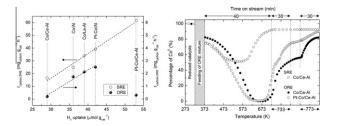
Jing Xu, Xin-Chao Xu, Like Ouyang, Xue-Jing Yang, Wei Mao, Junjie Su, Yi-Fan Han\*



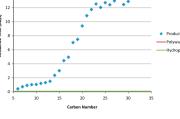
Mechanistic study of PROX of CO was carried out over a Pt(1.0 wt.%)/NAY zeolite catalyst from 300 to 523 K by combination of kinetics and spectroscopy. The activity of CO oxidation at 300 K was assumed to originate from Pt clusters less than 1.0 nm. In the presence of H<sub>2</sub>, a significant red-shift of the CO stretch frequency was observed in DRIFT spectra and CO oxidation was significantly enhanced.

#### Understanding the stability of Co-supported catalysts during ethanol reforming as addressed by in situ temperature pp 124-137 and spatial resolved XAFS analysis

C.N. Ávila-Neto, J.W.C. Liberatori, A.M. da Silva, D. Zanchet, C.E. Hori, F.B. Noronha, J.M.C. Bueno\*



Temperature- and spatial resolved XANES indicated that the nature of supports and the composition of reactants determine the Co<sup>2+</sup>/Co<sup>0</sup> ratio in reforming of ethanol, which control the activity and deposition of carbon.





pp 93-101



# Photocatalytic oxidation of ethanol and isopropanol vapors on cadmium sulfide

Maxim A. Nasalevich, Ekaterina A. Kozlova, Tatyana P. Lyubina, Alexander V. Vorontsov\*

$$\begin{split} & 2C_2H_5OH + O_2 \xrightarrow{-2h\nu}{cds} 2CH_3CHO + 2H_2O \\ & 2(CH_3)_2CHOH + O_2 \xrightarrow{-2h\nu}{cds} 2(CH_3)_2CO + 2H_2O \end{split}$$

Nanosized cadmium sulfide photocatalyzes partial oxidation of alcohol vapors with oxygen of air at room temperature under visible light with quantum efficiency up to 6.6%.

Nanosized cadmium sulfide photocatalyzes partial oxidation of alcohol vapors with oxygen of air at room temperature under visible light with quantum efficiency up to 6.6%.

# Controlled preparation and high catalytic performance of three-dimensionally ordered macroporous LaMnO<sub>3</sub> with pp 149–160 nanovoid skeletons for the combustion of toluene

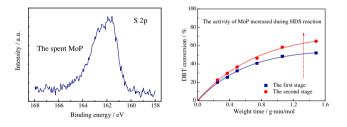
Yuxi Liu, Hongxing Dai\*, Yucheng Du, Jiguang Deng, Lei Zhang, Zhenxuan Zhao, Chak Tong Au

Dt-assisted PMMA-templating method, we prepared three-dimensionally ordered macroporous (3DOM) LaMpO- catalysts with

Through the surfactant-assisted PMMA-templating method, we prepared three-dimensionally ordered macroporous (3DOM) LaMnO<sub>3</sub> catalysts with nanovoid skeletons. It is found that the excellent performance of the catalysts in toluene combustion can be related to the high surface area and oxygen adspecies concentration as well as low-temperature reducibility of 3DOM LaMnO<sub>3</sub>.

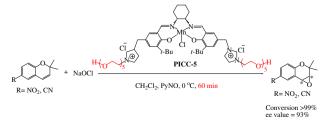
#### Hydrodesulfurization of dibenzothiophene and its hydrogenated intermediates over bulk MoP

Jin Bai, Xiang Li\*, Anjie Wang, Roel Prins, Yao Wang



# Stable chiral salen Mn(III) complexes with built-in phase-transfer capability for the asymmetric epoxidation of unfunctionalized olefins using NaOCI as an oxidant

Rongchang Luo, Rong Tan\*, Zhigang Peng, Weiguo Zheng, Yu Kong, Donghong Yin\*



PEG chain-modified ionic liquid functionalized chiral salen Mn(III) complexes with built-in phase-transfer capability were first prepared and proved highly efficient in the asymmetric epoxidation of unfunctionalized olefins using aqueous NaOCI as an oxidant.

#### pp 161-169

pp 170-177

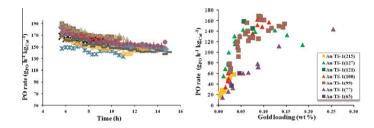
pp 138-148

# Reproducible preparation of Au/TS-1 with high reaction rate for gas phase epoxidation of propylene

Wen-Sheng Lee, M. Cem Akatay, Eric A. Stach, Fabio H. Ribeiro, W. Nicholas Delgass\*

#### pp 178-189

pp 190-202



The Au/TS-1 catalysts prepared at optimal DP conditions (pH of the gold slurry solution, the mixing time, and the preparation temperature) showed a PO rate  $\sim 160 \text{ g}_{PO}h^{-1}\text{kg}_{cat}^{-1}$ , which is the highest PO rate at 200 °C yet reported. Instead of using TS-1 with high Ti content to increase the site density, diluted systems (low Au loading/low Ti loading) are recommended for preparing highly active Au/TS-1 for PO production.

### Preferential oxidation of carbon monoxide in hydrogen using zinc oxide photocatalysts promoted and tuned by adsorbed copper ions

Yusuke Yoshida, Yu Mitani, Takaomi Itoi, Yasuo Izumi\*

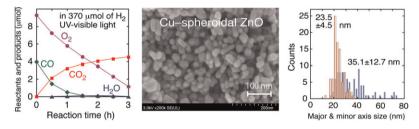
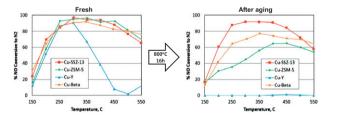


Photo-PROX: Preferential oxidation of CO in H<sub>2</sub> by photocatalysis using Cu(II) on spheroidal ZnO as the catalyst.

#### Effects of hydrothermal aging on NH<sub>3</sub>-SCR reaction over Cu/zeolites

Ja Hun Kwak\*, Diana Tran, Sarah D. Burton, János Szanyi, Jong H. Lee\*, Charles H.F. Peden\*



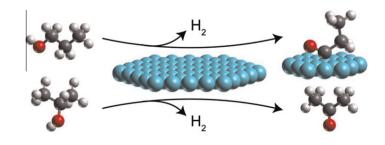
After hydrothermal aging at 800 °C for 16 h, the NOx reduction performance of Cu-ZSM-5, Cu-beta and Cu-Y were significantly reduced, while that of Cu-SSZ-13 was not affected.

#### LETTER TO THE EDITOR

Comment on "Towards understanding the bifunctional hydrodeoxygenation and aqueous phase reforming of glycerol" pp 210–213 [J. Catal. 269 (2010) 411–420]

Duygu Basaran, Alexander Genest, Notker Rösch

The experimentally observed dissimilar dehydrogenation behavior of 1- and 2- propanol on Pt surfaces is rationalized via DFT model calculations. The most stable dehydrogenation product of the primary alcohol, propionyl, strongly adsorbs whereas for the secondary alcohol, acetone is determined as product which desorbs easily.



pp 203-209