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### Journal of Molecular Catalysis A: Chemical

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#### **Contents**

#### Articles

#### Munir D. Khokhar, Ram S. Shukla, Raksh V. Jasra

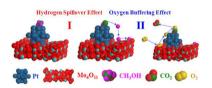
Journal of Molecular Catalysis A: Chemical 400 (2015) 1

Hydroformylation of dihydrofurans catalyzed by rhodium complex encapsulated hexagonal mesoporous silica • HRh(CO)(PPh<sub>3</sub>)<sub>3</sub>-HMS catalysed hydroformylation of 2,3and 2,5-dihydrofurans. • Conversion of 2,3-DHF was 98% with 89% selectivity of THF-2-carbaldehyde. • Conversion of 2,5-DHF was 90% with 72% selectivity of THF-3-carbaldehyde. • Conversion and selectivity depended on the catalyst amount and total pressure. • Catalyst was effectively recycled for both dihydrofurans.

#### Fan Yang, Fan Li, Yan Wang, Xin Chen, Dingguo Xia, Jingbo Liu

Journal of Molecular Catalysis A: Chemical 400 (2015) 7

Enhanced electrocatalytic performance for methanol oxidation with a Magnéli phase molybdenum oxide/ Pt-black composite • Crystallised Magnéli phase Mo<sub>4</sub>O<sub>11</sub> used as a co-catalyst support to enhance MOR. • Multiple Mo valence states coexist in Mo<sub>4</sub>O<sub>11</sub>. • These promote hydrogen spillover and oxygen buffering in the Pt/Mo<sub>4</sub>O<sub>11</sub> catalyst. • The catalyst shows improved poisoning tolerance and electrocatalytic activity



Schematic illustration of the synergistic effect of  $Pt/Mo_4O_{11}$  catalysing methanol oxidation reaction (MOR), including the hydrogen spillover effect and the oxygen buffering effect.

## Dong Wang, Christophe Deraedt, Jaime Ruiz, Didier Astruc

Journal of Molecular Catalysis A: Chemical 400 (2015) 14

Sodium hydroxide-catalyzed transfer hydrogenation of carbonyl compounds and nitroarenes using ethanol or isopropanol as both solvent and hydrogen donor

• Sodium hydroxide catalyze aryl ketone hydrogenation in ethanol at 80°C. • Sodium hydroxide reduces nitroarene to azoxyarene and azoarene in alcohols. • Selectivity in nitroarene reduction is strongly dependent on the alcohol structure.

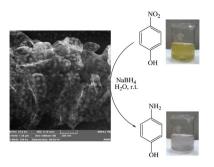
$$\begin{array}{c|c}
 & \text{NaOH} \\
\hline
 & \text{EtOH, 80°C}
\end{array}$$

#### Mahmoud Nasrollahzadeh, S. Mohammad Sajadi, Akbar Rostami-Vartooni, Mojtaba Bagherzadeh, Reza Safari

Journal of Molecular Catalysis A: Chemical 400 (2015) 22

Immobilization of copper nanoparticles on perlite: Green synthesis, characterization and catalytic activity on aqueous reduction of 4-nitrophenol

- Green synthesis of Cu NPs/perlite composite.
- Catalytic reduction of 4-nitrophenol to 4-aminophenol. • Catalyst was characterized using XRF, XRD, SEM, EDS, TEM, TG-DTA, BET, and FT-IR.
- Catalyst can be easily recovered and reused.



#### Liangfang Huang, Wenmin Wang, Haiyan Wei

Journal of Molecular Catalysis A: Chemical 400 (2015) 31

A computational study on high-valent mono-oxorhenium(V) complex-catalyzed hydrosilylation of carbonyls: What a difference an oxo ligand makes

•  $Re(O)Cl_3(PPh_3)_2$  catalyzed the hydrosilylation favoring an ionic pathway. • The [2+2] addition pathway is 11.1 kcal/mol higher than the ionic pathway. • The  $\sigma$ -bond metathesis pathway is 7.4 kcal/mol higher than the ionic pathway.

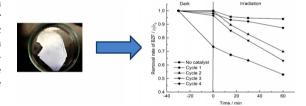


 $Re(O)Cl_3(PPh_3)_2$  acts as Lewis acid catalyzing the hydrosilylation of carbonyls.

#### Meijie Ren, Fritz H. Frimmel, Gudrun Abbt-Braun

Journal of Molecular Catalysis A: Chemical 400 (2015) 42

Multi-cycle photocatalytic degradation of bezafibrate by a cast polyvinyl alcohol/titanium dioxide (PVA/ TiO<sub>2</sub>) hybrid film • PVA/TiO<sub>2</sub> photocatalyst provided a highlyactive and recyclable catalyst for water purification. • The photocatalytic degradation efficiency increased with the increase of reuse cycle. • Technically the hybrid film was fairly stable under the long-term irradiation of the work.

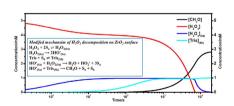


#### Miao Yang, Mats Jonsson

Journal of Molecular Catalysis A: Chemical 400 (2015) 49

Surface reactivity of hydroxyl radicals formed upon catalytic decomposition of H<sub>2</sub>O<sub>2</sub> on ZrO<sub>2</sub>

• Competition between  $H_2O_2$  and Tris for surfacebound HO• was quantified. • Competition is governed by the relative surface coverage. • Competition between  $O_2$  and  $H_2O_2$  for •  $CH_2OH$  (precursor for  $CH_2O$ ) was revealed. • Site-specific mechanism of  $H_2O_2$  decomposition on the surface of  $ZrO_2$  was proposed. • Numerical simulations reproduce the experimental results.



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