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Articles

M. Setnička, R. Bulánek, L. Čapek, P. Čičmanec

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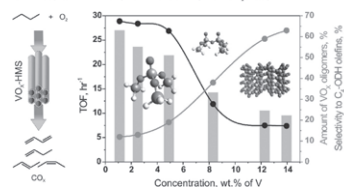
n-Butane oxidative dehydrogenation over VO_x-HMS catalysts

► VO_x units on mesoporous HMS were studied by means of analytic techniques. ► Monomeric VO_x units play role of most active and selective site in ODH of *n*-butane. ► Amount of monomeric units is comparable for synthesized and impregnated samples. ► Presence of O_n-oligomeric units causes decreasing of selectivity to C4-ODH products. ► Higher selectivity to C4-ODH products exhibit samples prepared by direct synthesis.

n-Butane oxidative dehydrogenation over VO_x-HMS catalyst

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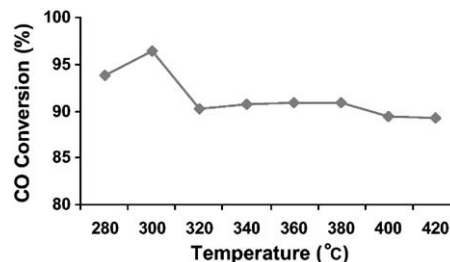


Ali Reza Salehi Rad, Maryam behzad khoshgouei, Ali Reza Rezvani

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Water gas shift reaction over Zn–Ni/SiO₂ catalyst prepared from [Zn(H₂O)₆]₂[Ni(NCS)₆]·H₂O/SiO₂ precursor

► The method of Zn–Ni/SiO₂ catalyst preparation is a simple and suitable way. ► The Zn–Ni catalyst has the high catalytic activity for WGS reaction at 280–420 °C. This catalyst presents higher activity than those prepared from other methods.

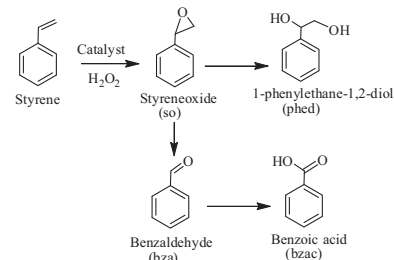


Mannar R. Maurya, Manisha Bisht, Fernando Vecilla

Journal of Molecular Catalysis A: Chemical 344 (2011) 18

Synthesis, characterization and catalytic activities of vanadium complexes containing ONN donor ligand derived from 2-aminoethylpyridine

► Synthesis and characterization of oxidovanadium(IV and V) complexes with new ligand derived from pyridoxal and 2-aminoethylpyridine (Hpydx-aepy). ► Structure of [V^{IV}O(acac)(pydx-aepy)] (1) has been solved by single crystal X-ray. ► Formation of the peroxido complex in solution has also been monitored by electronic absorption spectroscopy. ► Encapsulation of [V^{IV}O₂(pydx-aepy)] in the cavity of zeolite-Y and their catalytic activity for the oxidation of styrene, methyl phenyl sulfide, diphenyl sulfide and cyclohexene. ► Catalytic results are very good.

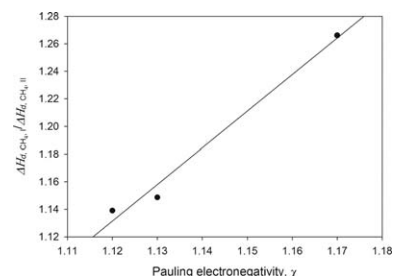


Say Yei Foo, Chin Kui Cheng, Tuan-Huy Nguyen, Adesoji A. Adesina

Journal of Molecular Catalysis A: Chemical 344 (2011) 28

Evaluation of lanthanide-group promoters on Co–Ni/Al₂O₃ catalysts for CH₄ dry reforming

► Lanthanide doping did not appear to affect CH₄ and CO₂ consumption rates. ► However, rare-earth promotion increased H₂ and CO production rates. ► Carbon deposition on the promoted catalysts reduced by up to 50%. ► Catalyst attributes correlated well with Pauling electronegativity of the dopants.

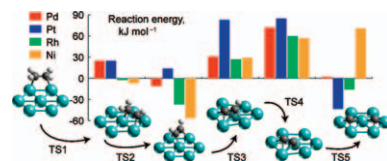


Duygu Basaran, Hristiyan A. Aleksandrov, Zhao-Xu Chen, Zhi-jian Zhao, Notker Rösch

Journal of Molecular Catalysis A: Chemical 344 (2011) 37

Decomposition of ethylene on transition metal surfaces M(1 1 1). A comparative DFT study of model reactions for M = Pd, Pt, Rh, Ni

► Theoretical study of ethylene decomposition on M(1 1 1) surfaces, M = Pd, Pt, Rh, Ni. ► Species with more H atoms dehydrogenate more easily than species with fewer H. ► Dehydrogenation occurs easier on Ni(1 1 1) and Rh(1 1 1) than on Pd(1 1 1) and Pt(1 1 1). ► Reactivity of Pd (Rh) regarding ethylene decomposition similar to that of Pt (Ni). ► Pd and Rh favor C₂ decomposition whereas on Ni C₂ formation is favored.

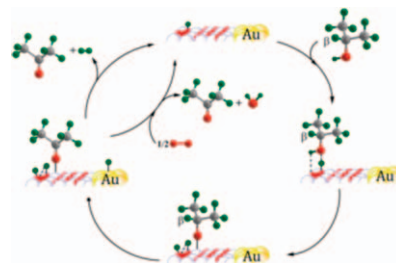


Z. Martinez-Ramirez, S.A. Jimenez-Lam, J.C. Fierro-Gonzalez

Journal of Molecular Catalysis A: Chemical 344 (2011) 47

Infrared spectroscopic evidence of adsorbed species during the oxidation of 2-propanol catalyzed by γ-Al₂O₃-supported gold: Role of gold as a hydrogen-subtractor

► γ-Al₂O₃-supported gold is catalytically active for the oxidation of 2-propanol. ► IR spectra of functioning catalysts identified species bonded to the support. ► Results suggest that the alcohol is activated on the support. ► Role of gold consists of subtracting hydrogen from β-C–H bond of surface alkoxide.

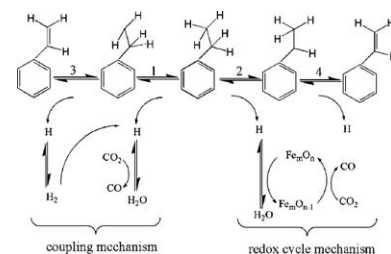


Xiao-Xiang He, Chen Fan, Xiong-Yi Gu, Xing-Gui Zhou, De Chen, Yi-An Zhu

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Role of CO₂ in ethylbenzene dehydrogenation over Fe₂O₃(0 0 1) from first principles

► The mechanism for ethylbenzene dehydrogenation in the presence of CO₂ is explored. ► Styrene is hard to escape from the most active O-terminated Fe₂O₃(0 0 1). ► The Fe-terminated surface dominates the reaction, with the coupling mechanism. ► Both the one-step and two-step pathways are probable while the former is dominant.

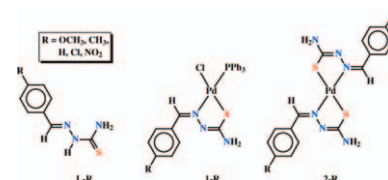


Piyali Paul, Sayanti Datta, Sarmistha Halder, Rama Acharyya, Falguni Basuli, Ray J. Butcher, Shie-Ming Peng, Gene-Hsiang Lee, Alfonso Castineiras, Michael G.B. Drew, Samaresh Bhattacharya

Journal of Molecular Catalysis A: Chemical 344 (2011) 62

Syntheses, structures and efficient catalysis for C–C coupling of some benzaldehyde thiosemicarbazone complexes of palladium

► Reaction of 4-R-benzaldehyde thiosemicarbazones with $[\text{Pd}(\text{PPh}_3)_2\text{Cl}_2]$ afford complexes (**1-R**) containing a thiosemicarbazone, a PPh_3 and a chloride. ► Similar reaction with $\text{Na}_2[\text{PdCl}_4]$ afford bis-thiosemicarbazone complexes (**2-R**). ► Coordination to Pd is associated with a conformational change around the C=N Bond. ► Both **1-R** and **2-R** complexes can efficiently catalyze C–C coupling reactions.

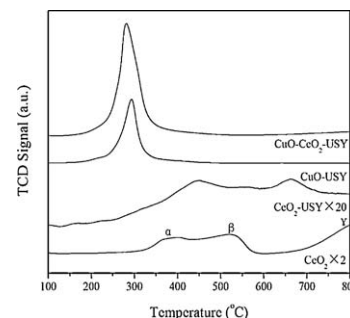


Qinqin Huang, Xiaomin Xue, Renxian Zhou

Journal of Molecular Catalysis A: Chemical 344 (2011) 74

Catalytic behavior and durability of CeO_2 or/and CuO modified USY zeolite catalysts for decomposition of chlorinated volatile organic compounds

► The catalytic activity for CVOCs destruction is evidently enhanced over modified USY catalysts. ► The high activity is due to high dispersion of CeO_2 or CuO , good oxygen mobility and Lewis acidity. ► Modified USY catalysts present high selectivity to HCl and CO_2 formation. ► Interaction between CuO and CeO_2 improves the durability of the catalyst in long term reaction.

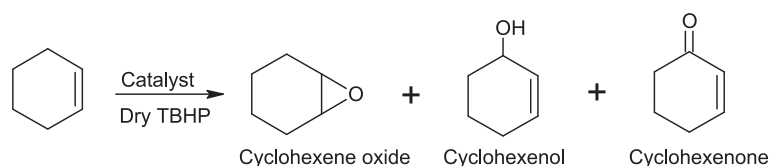


Savita Khare, Rajendra Chokhare

Journal of Molecular Catalysis A: Chemical 344 (2011) 83

Synthesis, characterization and catalytic activity of $\text{Fe}(\text{Salen})$ intercalated α -zirconium phosphate for the oxidation of cyclohexene

► Synthesis of a heterogeneous catalyst, α -ZrP-Fe(Salen) by flexible ligand method. ► Catalyst characterized by BET, XRD, SEM, EDX, FTIR, AAS and Mössbauer spectroscopy. ► Catalytic activation of α -ZrP-Fe(Salen) with dry TBHP for oxidation of cyclohexene. ► Study of recycling of the catalyst up to eight cycles.

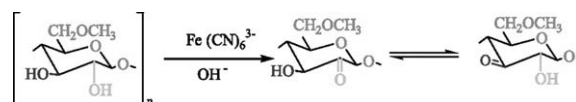


R.M. Hassan, S.M. Ibrahim, I.A. Zaafarany, A. Fawzy, H.D. Takagi

Journal of Molecular Catalysis A: Chemical 344 (2011) 93

Base-catalyzed oxidation: Kinetics and mechanism of hexacyanoferrate (III) oxidation of methyl cellulose polysaccharide in alkaline solutions

► A kinetic study of the oxidation of some natural polymeric compounds such as methyl cellulose polysaccharides by alkaline ferricyanide (III). ► A novel synthesis of diketo-derivatives of methyl cellulose by an oxidation method. ► Examining the behavior of polysaccharides containing alcoholic groups in aqueous alkaline solutions. ► Elucidation of reaction mechanism for the oxidation process of the cited work.

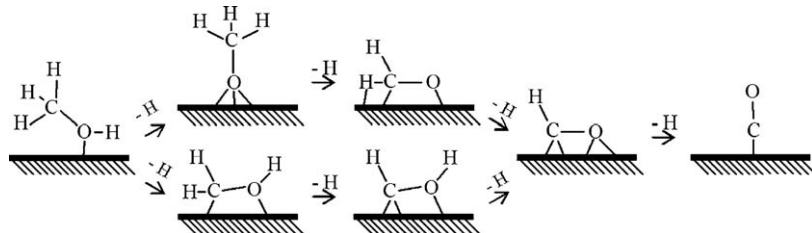


Ruibin Jiang, Wenyue Guo, Ming Li, Houyu Zhu, Lianming Zhao, Xiaqing Lu, Honghong Shan

Journal of Molecular Catalysis A: Chemical 344 (2011) 99

Methanol dehydrogenation on Rh(1 1 1): A density functional and microkinetic modeling study

► Rh(1 1 1)-catalyzed methanol dehydrogenation is studied using theory modeling. ► The reaction mechanism is identified under two different reaction conditions. ► The reason why oxidation does not take place at CH₂O in methanol oxidation is found. ► The origin of different mechanisms of the reaction on different VIII metals is found.

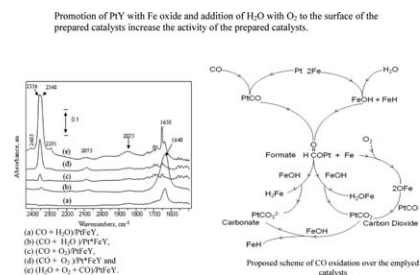


Zeinhom M. El-Bahy, Ahmed I. Hanafy, Mohamed M. Ibrahim, Masakazu Anpo

Journal of Molecular Catalysis A: Chemical 344 (2011) 111

In situ FTIR studies of CO oxidation over Fe-free and Fe-promoted PtY catalysts: Effect of water vapor addition

► Preparation and characterization of PtY and PtFeY catalysts by ion exchange method. ► In situ FTIR studies of CO oxidation, WGS over as prepared and reduced catalysts. ► Study the effect of addition of trace amount of water on the oxidation of CO with O₂. ► Addition of H₂O and/or H₂O + O₂ enhanced CO removal over Fe-free and Fe-promoted PtY. ► Admission of (CO + O₂ + H₂O) mixture increased the adsorbed amount of CO₂ over PtFeY.

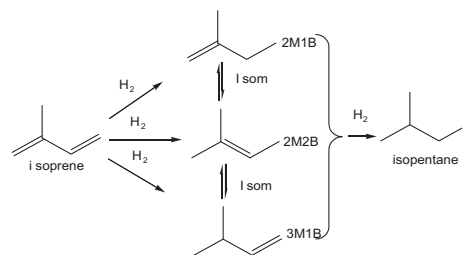


Rong Wang, Yonghong Li, Ronghui Shi, Meimei Yang

Journal of Molecular Catalysis A: Chemical 344 (2011) 122

Effect of metal–support interaction on the catalytic performance of Ni/Al₂O₃ for selective hydrogenation of isoprene

► The different metal–support interactions over two alumina supports were characterized. ► The effect of the different interaction on catalytic performance was explained. ► The weak interaction resisting coke deposition was related to the hydrogenolytic sites.

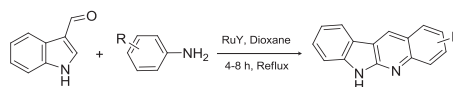


Alireza Khorshidi, Khalil Tabatabaeian

Journal of Molecular Catalysis A: Chemical 344 (2011) 128

Ruthenium-exchanged FAU-Y zeolite catalyzed improvement in the synthesis of 6H-indolo[2,3-b]quinolines

► A convenient method for preparation of indoloquinolines is reported. ► RuY as a heterogeneous catalyst resulted in more efficiency. ► Reusability of the solid acid catalyst is also, noticeable.

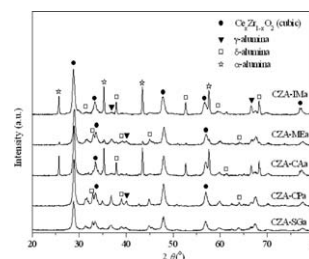


Qiyuan Wang, Zhenguo Li, Bo Zhao, Guangfeng Li, Renxian Zhou

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Effect of synthesis method on the properties of ceria-zirconia modified alumina and the catalytic performance of its supported Pd-only three-way catalyst

► The ceria-zirconia modified alumina (CZA) was prepared by five different methods. ► The effect of preparation methods on the structural properties of CZA was studied. ► Coprecipitation with supercritical drying leads to good thermal stability of CZA. ► The corresponding Pd-only three-way catalyst exhibits higher catalytic performance.

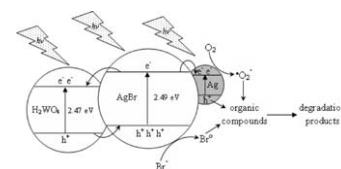


Jing Cao, Bangde Luo, Haili Lin, Shifu Chen

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Synthesis, characterization and photocatalytic activity of AgBr/H₂WO₄ composite photocatalyst

► AgBr/H₂WO₄ was synthesized by using a facile deposition-precipitation method. ► AgBr/H₂WO₄ displays excellent visible-light photocatalytic activity ($\lambda > 420$ nm). ► AgBr/H₂WO₄ possesses good stability after successive 5 cycle experiments. ► The resulting $\cdot\text{O}_2^-$, Br^0 and h^+ played the major roles for MO and RhB degradation.

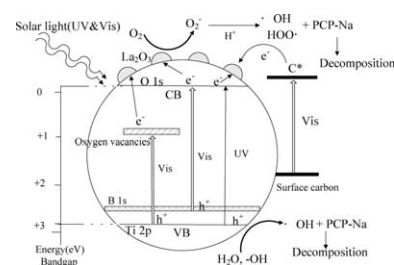


J.W. Liu, R. Han, H.T. Wang, Y. Zhao, W.J. Lu, H.Y. Wu, T.F. Yu, Y.X. Zhang

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Degradation of PCP-Na with La-B co-doped TiO₂ series synthesized by the sol-gel hydrothermal method under visible and solar light irradiation

► Novel La-B-TiO₂ synthesized by sol-gel hydrothermal route with high activity. ► Efficient decomposition and dechlorination of PCP-Na under visible and sun light. ► Synergetic effects of La and B implantation. ► Variation of catalytic activity with the action of the dopants in modified system.



Jo-Yong Park, Yun-Jo Lee, Prashant R. Karandikar, Ki-Won Jun, Jong Wook Bae, Kyoung-Su Ha

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Ru promoted cobalt catalyst on γ -Al₂O₃ support: Influence of pre-synthesized nanoparticles on Fischer-Tropsch reaction

► Controlled size CoRuO_x nanoparticles were embedded on γ -Al₂O₃. ► Intimate contact between Ru and Co increased by pre-synthesis of nanoparticles. ► 5CoRuAl catalysts show superior activity in Fischer-Tropsch reaction. ► Conventional catalyst with equal amount of Co and Ru show comparatively poor result. ► Increased interaction of Ru and Co in 5CoRuAl enhances catalyst activity.

