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Catalytic nanoreactors for ester hydrolysis

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Mild oxidation of hydrocarbons by *tert*-butyl hydroperoxide catalyzed by electron deficient manganese (III) corroles

Functional ionenes act as effective catalytic nanoreactors.
Alkaline hydrolysis of esters efficiently mediated by polysoaps.
Globular nanoreactors form hydrophobic microdomains.

Ana C. Coelho, Salete S. Balula, Margarida M. Antunes, Tsvetelina I. Gerganova, Nicolas Bion, Paula Ferreira, Martyn Pillinger, Anabela A. Valente, João Rocha, Isabel S. Gonçalves

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Complexation of crystal-like mesoporous phenylenesilica with $Cr(CO)_3$ and catalytic performance in the oxidation of cyclooctene ▶ Mesoporous phenylene-silica can be used as a support for metal carbonyl species. ▶ The liquid phase deposition of Cr(CO)₆ gives supported arenetricarbonyl complexes. ▶ The modified material promotes the catalytic epoxidation of cis-cyclooctene.
▶ In recycling runs the catalytic reaction is mainly heterogeneous in nature. ▶ A combination of free radical and non-radical reaction mechanisms may be involved.



PMO-C₆H₄Cr(CO)

CICH_CH_CI

40

20

S Substrate

-OH group in solution

lonene

-OH group attached to the ionene backbon



► Mn(III) corroles catalyze oxidation of hydrocarbons with *t*-BuOOH at room temperature. ► The catalytic

system proceeds through a radical-chain mechanism. ► The participation of ROO and ROOH has been proposed.





Hynek Balcar, David Bek, Jan Sedláček, Jiří Dědeček, Zdeněk Bastl, Martin Lamač

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 $RuCl_2(p$ -cymene)(PCy₃) immobilized on mesoporous molecular sieves as catalyst for ROMP of norbornene and its derivatives

RuCl₂(*p*-cymene)(PCy₃) (Cy = cyclohexyl) immobilized on mesoporous molecular sieves SBA-15 and MCM-41 exhibited high activity in ROMP of norbornene and its derivatives, providing high molecular weight polymers of low Ru content.



C. Amairia, S. Fessi, A. Ghorbel, A. Rîves

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Methane oxidation behaviour over sol-gel derived Pd/Al_2O_3 -ZrO₂ materials: Influence of the zirconium precursor

The zirconium precursor affects significantly the catalytic properties of Pd/Al₂O₃-ZrO₂ materials prepared by sol–gel method. Different catalytic behaviour has been observed when varying the zirconium precursor and content.



Haiqin Wan, Dan Li, Yue Dai, Yuhai Hu, Bin Liu, Lin Dong

Manganese oxide modified γ -Al₂O₃ could promote the dispersion capacity of CuO on this support because an epitaxil Mn₂O₃ monolayer formed on the γ -Al₂O₃ surface which results in the tetrahedral vacant sites of Mn₂O₃ to be preferentially occupied by Cu²⁺. The catalytic activities of CuO/ γ -Al₂O₃ for NO reduction by CO were improved by Mn₂O₃ modification because Cu⁺ formed in the Cu/Mn–Al catalysts.

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Catalytic behaviors of CuO supported on Mn_2O_3 modified γ -Al₂O₃ for NO reduction by CO



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Hydrocarbon selective catalytic reduction of NO over Cu/Fe-pillared clays: Diffuse reflectance infrared spectroscopy studies ▶ The first step for C_3H_6 -SCR over Cu-Fe-PILC is NO oxidation. ▶ The second step is propene adsorption on active sites. ▶ The third step is propene oxidation, promoted by CuO aggregates, to $C_xH_yO_z$. ▶ Next, $C_xH_yO_z$ reacts with NO_x to yield acetates or $C_xH_yO_z$ N compounds. ▶ Finally, the later species form N₂, CO₂ and H₂O as final products.



R.K. Sharma, Chetna Sharma

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A highly efficient synthesis of oxindoles using a functionalized silica gel as support for indium(III) acetylacetonate catalyst in an aqueous-acetonitrile medium

Yongna Zhang, Hongying Lü, Lu Wang, Yuliang Zhang, Peng Liu, Hongxian Han,

Zongxuan Jiang, Can Li

emulsion

Indium(III) acetylacetonate complex covalently anchored onto the surface of functionalized silica gel was found to be an efficient and recyclable catalyst in the synthesis of oxindoles derivatives.

► A series of emulsion catalysts were successfully synthesized. ► The catalyst with mono-lacunary structures shows high activity for BT oxidation. ► Metal-substituted catalysts show rather low activity for BT oxidation.



Sankaranarayanapillai Shylesh, Zhou Zhou, Qingguo Meng, Alex Wagener, Andreas Seifert, Stefan Ernst, Werner R. Thiel

type lacunary polytungstophosphate as catalysts in

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Sustainable, green protocols for heterogenized organocatalysts: N-Phenylthiazolium salts hybrid heterogenized on organic-inorganic mesoporous supports

A N-phenylthiazolium organocatalyst heterogenized on a mesoporous phenylene organosilica support shows superior catalytic activity, stability and reusability compared to a corresponding MCM-41 derived system in a series of organocatalytic reactions.



cat / 10 wt% H₂O:CH₃CN (4:1)

Oil phase

S.A. Patel, K.N. Patel, S. Sinha, B.V. Kamath, A.V. Bedekar

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Preparation of polymer anchored Pd-catalysts: Application in Mizoroki-Heck Reaction

▶ The present work deals with synthesis of polymer anchored Schiff bases and their complexes with PdCl2. The supports and catalysts are well characterized by usual techniques. The four catalysts prepared are screenedfor Mizoroki–Heck reaction with very good conversions and high TON, up to 88,000. ► The catalyst in the form of beads are easily separated and reused for 5 cycles for the same reaction. ► The Mizoroki-Heck reaction works better with iodoarenes than bromoarenes, and is ineffective for chloroarenes. A number of

reactions with combination of styrenes and aryl halides has been studied with good catalytic activity. ► The catalysts are very easy to synthesize, purify and are stable in air and water. The Mizoroki-Heck reaction is also done in water as environment friendly solvent.



Sunyoung Park, Dong Ryul Park, Jung Ho Choi, Tae Jin Kim, Young-Min Chung, Seung-Hoon Oh, In Kyu Song

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Direct synthesis of hydrogen peroxide from hydrogen and oxygen over insoluble $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ heteropolyacid supported on Pd/MCF

► Direct synthesis of hydrogen peroxide from hydrogen and oxygen was conducted. ► $Cs_{2,5}H_{0,5}PW_{12}O_{40}/Pd/MCF$ catalysts were used. ► Acidity of $Cs_{2,5}H_{0,5}PW_{12}O_{40}/Pd/$ MCF played an important role. ► Yield for hydrogen peroxide increased with increasing acidity of the catalyst.



Song Liu, Jiantao Wu, Xingping Liu, Rongying Jiang

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TiO₂/V–TiO₂ composite photocatalysts with an n–n heterojunction semiconductor structure

► $TiO_2/V-TiO_2$ composite photocatalysts exhibited high activity. ► Ammonium oleate was used to improve the structure of n-n heterojunction. ► The energy-band diagrams of $TiO_2/V-TiO_2$ composite photocatalysts were presented. ► A hypothetical configuration of composite photocatalysts was proposed.

support with regard to the unsupported Ru system.



Salah A. Hassan, Fatma Z. Yehia, Hamdi A. Hassan, Salwa A. Sadek, Atef S. Darwish

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Various characteristics and catalytic performance of iron (II) phthalocyanine immobilized onto titaniaand vanadia-pillared bentonite clay in *in situ* polymerization of methyl methacrylate. An attempt to synthesize novel polymer/iron phthalocyanine/ pillared clay nanocomposites ► Characterization of the modified bentonite, viz., through acid thermal treatment (ATTB) and by pillaring with titania and vanadia (Ti-PILB and V-PILB), as well as the hybrid catalytic system of Fe (II) phthalocyanine (FePc) immobilized onto modified clay samples (in 0.5 wt%, of diluted loading region). ► Following up catalytic performance of these systems in the *in situ* polymerization of MMA at 60 °C, in absence of a cocatalyst, aiming to elucidate the competing roles played by the complex, the pillars and the interlayer sites in the reaction mechanism, compared with other phthalocyanine systems. ► An attempt to synthesize novel PMMA/FePc (compatibilizer)/pillared clay (filler) nanocomposites, as polymerization end products.



► A bifunctional ligand leads to small and well-dispersed ruthenium nanoparticles. ► Functionalized multi-

walled carbon nanotubes efficiently immobilize ruthenium nanoparticles. Beneficial catalytic effect of the

Mohamad Jahjah, Yolande Kihn, Emmanuelle Teuma, Montserrat Gómez

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Ruthenium nanoparticles supported on multi-walled carbon nanotubes: Highly effective catalytic system for hydrogenation processes



Puttaswamy, Anu Sukhdev, J.P. Shubha

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Palladium(II)-catalyzed oxidation of tranexamic acid by bromamine-B in alkaline medium and uncatalyzed reaction in acid medium: A study of kinetic and mechanistic chemistry The present research investigation is the first report on the TA-BAB redox system from the kinetic and mechanistic points of view. ► The stoichiometry and oxidation products of TA by BAB in acid and alkaline media are the same, but their kinetic characteristics are different. ► Reactions of TA with BAB are 10-fold faster in acid medium in comparison with alkaline medium.
► Pd(II) catalyzed reactions in alkaline medium are found to be 6-fold faster than the uncatalyzed reactions.

$$Rate = \frac{K_I K_2 k_3 [BAB]_t [TA]}{[H^+] + K_I + K_I K_2 [TA]}$$
(1)
$$Rate = \frac{K_5 k_6 [BAB]_t [OH^-] [Pd(II)]}{(2)}$$
(2)

$$ate = \frac{(2)}{[H_2O] + K_S[OH^{-}]}$$

Zinaida P. Pai, Dimitry I. Kochubey, Polina V. Berdnikova, Vladislav V. Kanazhevskiy, Irina Yu. Prikhod'ko, Yuriy A. Chesalov

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Structure and properties of tungsten peroxopolyoxo complexes – Promising catalysts for organics oxidation. I. Structure of peroxocomplexes studied during the stepwise synthesis of tetra (diperoxotungsten) phosphate-tetra-n-butyl ammonium Catalysis via metal complexes has been studied using EXAFS and Raman spectroscopy. Main polyoxo- and peroxopolyoxocomplexes of tungsten, resulting from the interaction of phosphorus tungsten heteropolyacid with hydrogen peroxide in water solutions, were investigated with regard to their form and structure. Interaction was shown to reduce the nuclearity of forming complexes with respect to their precursor – $H_3PW_{12}O_{40}$. The symmetry of oxygen environment of tungsten was found to change, distances W–W remaining the same. After complex $[Bu^n_4N]_3[PO_4[WO(O_2)_2]_4]$ is isolated, binuclear anion $[W_2O_3(O_2)_4(H_2O_2)_2]^{2-}$ stays in the solution. Raman scattering, EXAFS and IR spectroscopy show that isolated peroxocomplex in its crystal state has four nuclei, and most probably retains this structure being dissolved in acetonitrile. Synthesized catalytic complex $[Bu^n_4N]_3[PO_4[WO(O_2)_2]_4]_4$ was

tested in oxidation of cyclic alkenes and alcohols with hydrogen peroxide. Complex $[Bu_{14}^nN]_3$ {PO₄ $[WO(O_2)_2]_4$ } was proved to provide higher yields of mono- and dicarbonic acids in comparison to *in situ* synthesized catalyst.



P. Veerakumar, Zong-Zhan Lu, M. Velayudham, Kuang-Lieh Lu, S. Rajagopal

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Alumina supported nanoruthenium as efficient heterogeneous catalyst for the selective H_2O_2 oxidation of aliphatic and aromatic sulfides to sulfoxides

▶ The work presented in this manuscript involves the synthesis and characterization of ruthenium nanoparticles and their application as catalyst for sulfoxidation reactions. ▶ This appears to be the first report on the oxidation of organic sulfides using ruthenium nanoparticles as catalyst. This is a simple and efficient system for the selective oxidation of sulfides to sulfoxides using H₂O₂, a green reagent, as the oxidant. ▶ Because it is a simple, convenient and novel method for the oxidation of sulfides using nanoruthenium as the catalyst. ▶ The heterogeneous catalysis on the H₂O₂ oxidation of sulfides in the presence of catalyst I, which is one of the most convenient, cheap and green methods for the synthesis of various sulfoxides. ▶ Aqueous H₂O₂ is an ideal oxidant owing to its high effective-oxygen content, cleanliness (it produces only water as by-product), and enough safety in storage and operation. Therefore, H₂O₂ is important as a "green" oxidizing agent.



R.M. Hassan, A. Alaraifi, A. Fawzy, I.A. Zaafarany, K.S. Khairou, Y. Ikeda, H.D. Takagi

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Acid-catalyzed oxidation of some sulfated polysaccharides. Kinetics and mechanism of oxidation of kappa-carrageenan by cerium(IV) in aqueous perchlorate solutions ► The kinetics of oxidation of some sulfated macromolecules in acidic solutions by cerium(IV) ion. ► Novel synthesis of keto-acid derivatives of kappa-carrageenan by an oxidation process. ► Behavior of sulfated polysaccharides in aqueous acidic solutions. ► Elucidation of reaction mechanistics for the oxidation.



Xiaowa Nie, Xin Liu, Chunshan Song, Xinwen Guo

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Brønsted acid-catalyzed tert-butylation of phenol, *o*-cresol and catechol: A comparative computational study ► DFT calculations provide new insight into tert-butylation mechanisms. ► The differences in the stability of O-alkylation intermediates account for the regioselectivity to tert-butyl ether from phenolics. ► The intramolecular H-bond inhibits tert-butyl ether formation from catechol.



Zhenjin Xu, Hui Wan, Jinmei Miao, Mingjuan Han, Cao Yang, Guofeng Guan

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Reusable and efficient polystyrene-supported acidic ionic liquid catalyst for esterifications

▶ Polystyrene (PS)-supported 1-(propyl-3-sulfonate) imidazolium hydrosulfate acidic ionic liquid (PS-CH₂-[SO₃H-pIM][HSO₄]) catalyst was prepared. ▶ The prepared PS-CH₂-[SO₃H-pIM][HSO₄] catalyst was used for esterifications with high yields. ▶ The PS-CH₂-[SO₃HpIM][HSO₄] catalyst could be recovered by simple filtration, and the yield only decreased 7.3% for the synthesis of n-butyl acetate after reusing for 13 times.



Andrea Vavasori, Federico Dall'Acqua, Gianni Cavinato, Luigi Toniolo

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Influence of the operating conditions on the catalytic activity of $[PdCl_2(dapp)]$ in the CO-ethene copolymerization in the H_2O-CH_3COOH as a solvent (dapp = 1,3-bis(di(2-methoxyphenyl) phosphino) propane)

▶ [PdCl₂(dapp)] catalyzes the CO–ethene copolymerization in H₂O–AcOH as a solvent. ▶ At 90 °C, 110 atm (CO/E 1/1), H₂O 55%, 22,800 g PK(g Pd h)⁻¹ are achieved, LVN 3.8 dL/g. ▶ At 60 °C 2500 g PK(g Pd h)⁻¹ are produced with a much higher LVN (11.2 dL/g). ▶ At 75 °C both productivity and LVN are relatively high, 15,000 g PK(g Pd h)⁻¹, 7 dL/g.

n == + n CO + H₂O -[Pd] = [PdCl_(dapp)]

solv. = H2O-AcOH