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Contents

Unexpected phosphate salt-catalyzed hydrolysis of glycosidic bonds in model disaccharides: Cellobiose and maltose pp 1–5 Alexandre Charmot, Alexander Katz*



Glycosidic bond hydrolysis in both cellobiose and maltose proceeds under unexpectedly mild conditions when using simple phosphate salts as catalyst.

Role and advantages of H₂S in catalytic steam reforming over nanoscale CeO₂-based catalysts

N. Laosiripojana*, S. Charojrochkul, P. Kim-Lohsoontorn, S. Assabumrungrat



Unlike conventional metallic-based catalysts, the presence of poisonous H_2S gas (with appropriate content) increases the steam reforming rate of CeO₂-based catalysts, which is related to the formation of Ce(SO₄)₂ phase during the reaction.

Determination of active site densities and mechanisms for soot combustion with O2 on Fe-doped CeO2 mixed oxidespp 16-23Zhaoliang Zhang*, Dong Han, Shaojie Wei, Yexin ZhangPhane CeO2 mixed oxidesPhane CeO2 mixed oxides

Soot O-Fe³⁺ O-Fe²⁺ O-Fe³⁺ O-Ce⁴⁺ O O-Fe³⁺ O-Ce⁴⁺ O O-Fe³⁺ O-Ce⁴⁺ O O-Ce⁴⁺ O O-Ce³⁺ O-Ce

The densities of active oxygen sites and turnover frequencies for soot combustion on Fe-doped CeO₂ mixed oxides are determined by isothermal anaerobic titrations with soot as the probe molecule.

pp 6-15

Stability and performance of cation vacant $Fe_{3-x-v}V_x \Box_v O_4$ spinel phase catalysts in methanol oxidation

pp 38-48

Robert Häggblad, Staffan Hansen, L. Reine Wallenberg, Arne Andersson*



Cation vacant spinel phases with V-sites surrounded by Fe (V-O-Fe) are stable, active, selective and non-volatile in methanol oxidation to formaldehyde.

TAP studies of CO oxidation over CuMnO_X and Au/CuMnO_X catalysts

Kevin Morgan, Kieran J. Cole, Alexandre Goguet, Christopher Hardacre*, Graham J. Hutchings, Noleen Maguire, Sergiy O. Shekhtman, Stuart H. Taylor



TAP studies of the CO oxidation reactions over CuMnOx (Hopcalite) catalysts has revealed that the increased activity on doping with gold is due to promotion of the Mars van Krevelen mechanism with little change in the activity associated with the Langmuir-Hinshelwood mechanism.

Investigating the mechanism of the H₂-assisted selective catalytic reduction (SCR) of NOx with octane using fast cycling pp 49-55 transient in situ DRIFTS-MS analysis

Sarayute Chansai, Robbie Burch, Christopher Hardacre*, John Breen, Frederic Meunier



Examination of the H2-assisted Selective Catalytic Reduction of NO_x with octane over a Ag/Al₂O₃ catalyst using fast transient cycling switching of H₂, monitored by DRIFTS and mass spectrometry, suggests that some of the isocyanate species could be important intermediates in this reaction.

Cr-MnO_x mixed-oxide catalysts for selective catalytic reduction of NO_x with NH₃ at low temperature

pp 56-65

Zhihang Chen, Qing Yang, Hua Li, Xuehui Li*, Lefu Wang, Shik Chi Tsang**



Impressive activity for low-temperature SCR of NOx is achieved on novel catalysts containing CrMn_{1.5}O4 phase, which provides catalytically active sites due to facilitated electron transfer between Cr and Mn.

The formation of methane over iron catalysts applied in Fischer–Tropsch synthesis: A transient and steady state kinetic pp 66–75 study

Barbara Graf, Hendrik Schulte, Martin Muhler*



CH₄ formation over unpromoted and potassium-promoted iron catalysts applied in Fischer–Tropsch synthesis was studied via hydrogenation of CO during pulse experiments. The presence of potassium influences CH₄ formation by blocking the fast formation channel at least partially and establishing a new and slower reaction pathway.

Copper-catalyzed propylene epoxidation by oxygen: Significant promoting effect of vanadium on unsupported copper pp 76–84 catalyst

Lüjuan Yang, Jieli He, Qinghong Zhang, Ye Wang*

Modification of unsupported copper by vanadium significantly enhances its catalytic activity for propylene epoxidation. Cu¹ with cooperation of vanadium species at lower valance states is responsible for propylene oxide formation.

Kinetic analysis of cluster size dependent activity and selectivity

Dmitry Yu. Murzin



The impact of nanoparticle size effects in heterogeneous catalytic kinetics over supported metal catalysts is discussed taking into account different activities of edges and terraces.

Descriptors controlling the catalytic activity of metallic surfaces toward water splitting

José L.C. Fajín, M. Natália D.S. Cordeiro, Francesc Illas*, José R.B. Gomes*

| $H_2O^* + * \rightarrow [HO^* \cdots H^*] \rightarrow HO^* + H^*$ | | | |
|---|----|----|----|
| | Со | Ni | Cu |
| Ru | Rh | Pd | Ag |
| | Ir | Pt | Au |
| decreasing reactivity | | | |

Water dissociation on regular, stepped and folded transition metal surfaces follows a BEP relationship. In addition, the adsorption energy of atomic oxygen on a given metallic surface provides an excellent descriptor of the activation energy thus allowing the screening of a large number of metallic and bimetallic systems in a simple way.

pp 85-91

pp 92-100

Steam reforming of methanol on PdZn near-surface alloys on Pd(1 1 1) and Pd foil studied by *in-situ* XPS, LEIS and pp 101–113 PM-IRAS

Christoph Rameshan, Christian Weilach, Werner Stadlmayr, Simon Penner, Harald Lorenz, Michael Hävecker, Raoul Blume, Tulio Rocha, Detre Teschner, Axel Knop-Gericke, Robert Schlögl, Dmitry Zemlyanov, Norbert Memmel, Günther Rupprechter, Bernhard Klötzer*



The bifunctional sites for methanol reforming on a multi- and monolayer Pd–Zn surface are structurally different, despite identical surface composition. The multilayer alloy activates water for reaction to CO₂ and H₂.

Kinetic characterization of unsupported ReS₂ as hydroprocessing catalyst

T.C. Ho*, Q. Shen, J.M. McConnachie, C.E. Kliewer

pp 114-122



Shown here are adsorption constants for 4,6-diethyldibenzothiophene (46DEDBT) and 3-ethylcarbazole (3EBZ) and hydrodenitrogenation rate constants on sulfided CoMo/Al₂O₃-SiO₂ and ReS₂. ReS₂ is more active for HDN; its HDS activity is less resilient to 3ECBZ inhibition.

Three-dimensional cubic mesoporous materials with a built-in N-heterocyclic carbene for Suzuki–Miyaura coupling of pp 123–133 aryl chlorides and C(sp³)-chlorides

Hengquan Yang*, Guang Li, Zhancheng Ma, Jianbin Chao, Zhiqiang Guo



New mesoporous hybrid materials with a built-in N-heterocyclic carbene in the framework were synthesized. Such materials are active and recyclable for Suzuki–Miyaura coupling of challenging aryl/benzylic chlorides.

Bridging homogeneous and heterogeneous catalysis with MOFs: "Click" reactions with Cu-MOF catalysts

pp 134-140

I. Luz, F.X. Llabrés i Xamena, A. Corma*



Copper-containing metal organic frameworks are highly active and fully regioselective heterogeneous "click" catalysts, with performances comparable to homogeneous Cu catalysts.

Transient mechanistic study of the gas-phase HCl oxidation to Cl₂ on bulk and supported RuO₂ catalysts Miguel A.G. Hevia, Amol P. Amrute, Timm Schmidt, Javier Pérez-Ramírez*

HCl 02 HC

Temporal Analysis of Products (TAP) reactor studies improve the mechanistic understanding of the gas-phase HCl oxidation to Cl₂ (Deacon process) over RuO₂-based catalysts.

Catalytic properties in polyolefin cracking of hierarchical nanocrystalline HZSM-5 samples prepared according to pp 152–160 different strategies

D.P. Serrano, J. Aguado*, J.M. Escola, J.M. Rodriguez, A. Peral

Hierarchical nanocrystalline ZSM-5 materials, prepared by a seed silanization method, showed a remarkable enhancement of the catalytic activity in the cracking of polyolefins compared to hierarchical ZSM-5 samples synthesized by a low-temperature procedure, the differences being especially pronounced for the case of waste polyethylene conversion.

A novel approach towards solvent-free epoxidation of cyclohexene by Ti(IV)–Schiff base complex-intercalated LDH using $pp 161-169 H_2O_2$ as oxidant

K.M. Parida*, Mitarani Sahoo, Sudarshan Singha



The solvent-free epoxidation reaction of cyclohexene using Ti-Schiff base complex-immobilized LDH will help experimentalist to achieve greener and most sustainable process.

Mesoporous mordenites obtained by sequential acid and alkaline treatments – Catalysts for cumene production with pp 170–180 enhanced accessibility

Adri N.C. van Laak, Sophia L. Sagala, Jovana Zečević, Heiner Friedrich, Petra E. de Jongh, Krijn P. de Jong*



Commercially available mordenite was subjected to post-synthesis treatments. Sequential acid and alkaline treatments were found to be most effective to obtain mesoporous mordenite and visualized with electron tomography. Mesoporous mordenite was close in activity to zeolite beta for the production of cumene, with superior selectivity toward the undesired *n*-propylbenzene.

pp 141-151

Solid acid catalysts based on $H_3PW_{12}O_{40}$ heteropoly acid: Acid and catalytic properties at a gas-solid interface

Ali M. Alsalme, Paul V. Wiper, Yaroslav Z. Khimyak, Elena F. Kozhevnikova, Ivan V. Kozhevnikov*

pp 181-189



The strength of acid sites of supported $H_3PW_{12}O_{40}$ (HPW) catalysts (enthalpy of NH_3 adsorption) is weaker, and their catalytic activity in isopropanol dehydration (TOF) is lower than those of the standard unsupported catalysts (bulk HPW and $Cs_{2.5}H_{0.5}PW_{12}O_{40}$); they decrease in the order of supports: $SiO_2 > TiO_2 > Nb_2O_5 > ZrO_2$ (all catalysts calcined at 300 °C).

On the understanding of the remarkable activity of template-containing mesoporous molecular sieves in the transesterification of rapeseed oil with ethanol

pp 190-196

Demian Patrick Fabiano, Berna Hamad, Dilson Cardoso, Nadine Essayem*



Template-containing molecular sieves such as [CTA]Si-MCM-48 were shown to possess very weak basic sites by calorimetry, however the CO₂ adsorption isotherms are totally reversible. Their catalytic activities in transesterification are comparable to that of strong inorganic bases.