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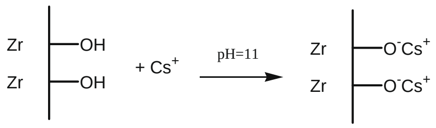
Contents

PRIORITY COMMUNICATION

Zirconia modified by Cs cationic exchange: Physico-chemical and catalytic evidences of basicity enhancement **pp 1–4**

Berna Hamad, Alain Perard, François Figueras, Franck Rataboul, Swamy Prakash, Nadine Essayem *

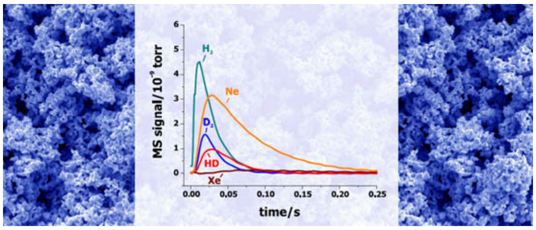


Zirconia promoted with Cs was prepared by cationic exchange of zirconium hydroxide with Cs, then calcined, and refluxed in ethanol to remove weakly bonded Cs species. The promotion with Cs stabilized the ZrO_2 tetragonal phase and has significantly increased the amount and the strength of the basic sites. In vegetable oil transesterification, TOFs higher than those of ZrO_2, MgAl-HDT, and NaOH were achieved over ZrOCs, demonstrating the potential of this novel solid base.

REGULAR ARTICLES

Activation of dihydrogen on supported and unsupported silver catalysts **pp 5–14**

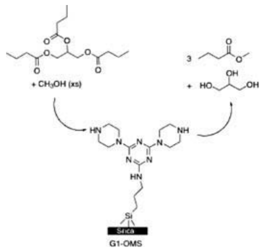
J. Hohmeyer, E.V. Kondratenko, M. Bron, J. Kröhnert, F.C. Jentoft, R. Schlögl, P. Claus *



H_2 activation on silver was investigated by temporal analysis of products (TAP), IR spectroscopy, and calorimetry. H_2 adsorption on silver catalysts is found to be activated. Activated hydrogen becomes available also on the surrounding support.

Catalytic properties of dendron–OMS hybrids **pp 15–25**

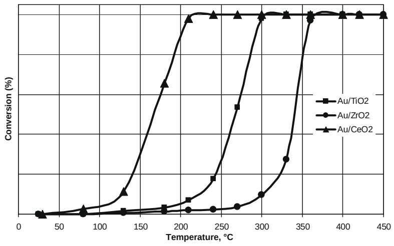
Qingqing Wang, Victor Varela Guerrero, Anirban Ghosh, Seunguk Yeu, Jonathan D. Lunn, Daniel F. Shantz *



Dendron–OMS hybrids have been investigated as catalysts and show promising reactivity and stability in the Henry reaction, transesterification of triglycerides, and the Aldol condensation of 5-(hydroxymethyl)furfural with acetone. These materials hold great promise as solid base catalysts.

Role of support in the oxidation of acetylene over gold catalysts pp 26–32

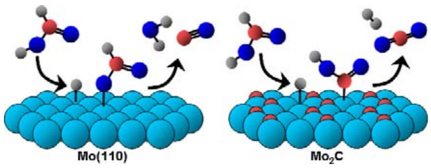
Yassine Azizi, Corinne Petit, Véronique Pitchon *



The influence of the carrier (CeO_2, TiO_2 or ZrO_2) on the reaction of acetylene oxidation over a 2% gold catalyst has been investigated in the presence or in the absence of CO. The differences in activities are explained. The reason lies in a different kinetic behaviour, mainly for the mode of adsorption and/or reaction of oxygen.

Selective decomposition of formic acid on molybdenum carbide: A new reaction pathway pp 33–43

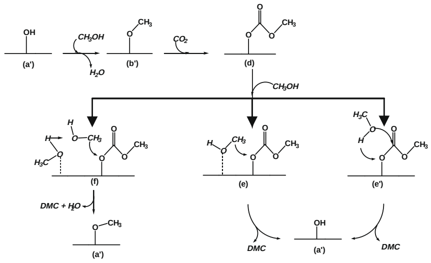
David W. Flaherty, Sean P. Berglund, C. Buddie Mullins *



Mo_2C is up to 15 times more selective towards formic acid dehydrogenation than Mo. Suppressed C–O bond dissociation leading to the formation of monodentate formate and carboxyl is responsible.

Influence of Al_2O_3 on the performance of CeO_2 used as catalyst in the direct carboxylation of methanol to dimethylcarbonate and the elucidation of the reaction mechanism pp 44–52

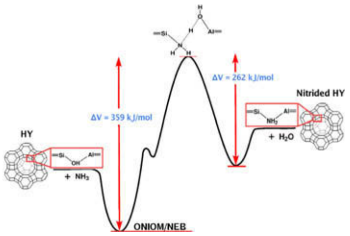
Michele Aresta *, Angela Dibenedetto, Carlo Pastore, Antonella Angelini, Brunella Aresta, Imre Pápai



The reaction mechanism for the carboxylation of methanol to dimethylcarbonate has been elucidated by using DRIFT and solid state and solution multinuclear NMR spectroscopy. Modified ceria catalysts perform better than ceria.

DFT study of nitrided zeolites: Mechanism of nitrogen substitution in HY and silicalite pp 53–63

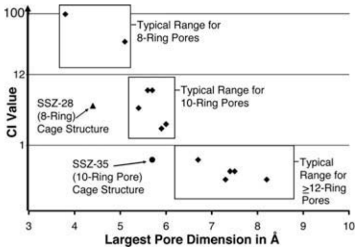
Vishal Agarwal, George W. Huber, W. Curtis Conner Jr., Scott M. Auerbach *



The mechanism of nitridation in HY and silicalite is revealed using denstiy functional theory. The barriers for forward and backward processes are large, indicating that nitrided zeolites are stable once formed.

Further investigations on Constraint Index testing of zeolites that contain cages pp 64–70

John R. Carpenter, Sheila Yeh, Stacey I. Zones, Mark E. Davis *



External surface activity and increased internal space are investigated to understand the low Constraint Index results compared to the pore size of SSZ-25 and SSZ-35, zeolites with large internal cages.

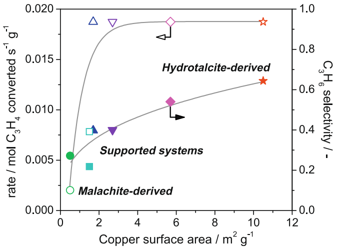
Small-sized HZSM-5 zeolite as highly active catalyst for gas phase dehydration of glycerol to acrolein pp 71–79

Chun-Jiang Jia, Yong Liu, Wolfgang Schmidt, An-Hui Lu, Ferdi Schüth *

The catalytic behavior of nanocrystalline HZSM-5 catalyst with a Si/Al ratio of 65 was studied in the gas phase dehydration of aqueous glycerol. Compared with bulk HZSM-5, the small-sized catalyst exhibits greatly enhanced catalytic performance in glycerol dehydration even at very high GHSV = 1438 h^{-1}.

Partial hydrogenation of propyne over copper-based catalysts and comparison with nickel-based analogues pp 80–92

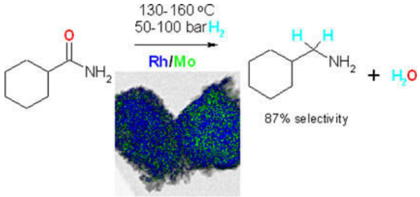
Blaise Bridier, Núria López, Javier Pérez-Ramírez *



Copper-based catalysts derived from activation of the Cu–Al hydrotalcite precursor display remarkable performance in the partial hydrogenation of propyne owing to the attainment of a high metal loading and a high copper dispersion. The reaction mechanism and product distribution present marked differences in comparison with nickel-based analogues.

Selective hydrogenation of amides using Rh/Mo catalysts pp 93–102

Graham Beamson, Adam J. Papworth, Charles Philipps, Andrew M. Smith, Robin Whyman *

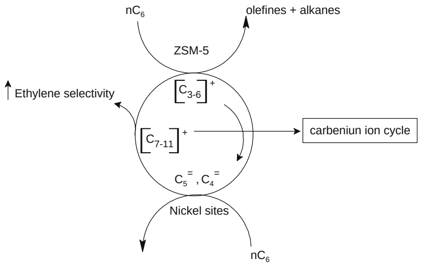


Selective reduction of amides to the corresponding amines has been achieved using recyclable, bimetallic heterogeneous Rh/Mo catalysts derived from $Rh_6(CO)_{16}$ and $Mo(CO)_6$. Primary amide substrates do *not* require the addition of ammonia to inhibit secondary amine formation.

Ni-ZSM-5 catalysts: Detailed characterization of metal sites for proper catalyst design

pp 103–109

A.J. Maia, B. Louis, Y.L. Lam, M.M. Pereira *

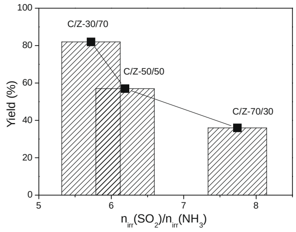


Nickel was introduced in ZSM-5 zeolite by two different methods: dry impregnation and ionic exchange. The catalytic activity of Ni-doped ZSM-5 zeolites was tested in n-hexane cracking. It was possible to modify the n-hexane cracking activity and selectivity toward light alkenes, by tailoring both the metallic and acidic active sites.

Knoevenagel condensation reaction over acid–base bifunctional nanocrystalline $Ce_xZr_{1-x}O_2$ solid solutions

pp 110–121

Georgeta Postole, Biswajit Chowdhury *, Bikash Karmakar, Kumari Pinki, Julie Banerji, Aline Auroux *

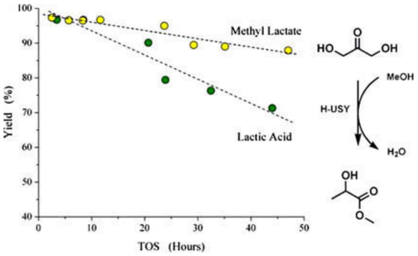


Knoevenagel condensation reaction on ceria–zirconia (C/Z) catalysts was studied in the liquid phase to probe effects of acid-basic character of these materials on their catalytic and structural properties. No evident correlation was found between catalytic performances and the basic character of the samples, but the catalytic activity was clearly influenced by the ratio of basic to acidic sites. Lower basic to acidic sites ratio led to higher product yield.

Zeolite H-USY for the production of lactic acid and methyl lactate from C_3-sugars

pp 122–130

Ryan M. West, Martin Spangsberg Holm, Shunmugavel Saravanamurugan, Jianmin Xiong, Zachary Beversdorf, Esben Taarning *, Claus Hviid Christensen

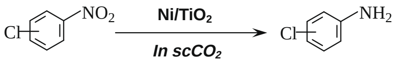


Conversion of dihydroxyacetone and glyceraldehyde to methyl lactate can be achieved in close to quantitative yields using commercially available acidic zeolites. The stability and rate of reaction was found to increase significantly by the use of methanol as solvent when compared to water.

Selective hydrogenation of chloronitrobenzene to chloroaniline in supercritical carbon dioxide over Ni/TiO_2: Significance of molecular interactions

pp 131–139

Xiangchun Meng, Haiyang Cheng, Shin-ichiro Fujita, Yufen Hao, Yanjiao Shang, Yancun Yu, Shuxia Cai, Fengyu Zhao *, Masahiko Arai *

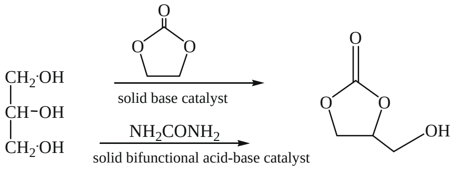


No accumulation of harmful intermediates and
negligible dechlorination at any conversion

The chemoselective hydrogenation of chloronitrobenzene to chloroaniline can be achieved at any conversion levels up to 100% over Ni/TiO_2 in $scCO_2$ at 35 °C.

Chemicals from biomass: Synthesis of glycerol carbonate by transesterification and carbonylation with urea with hydrotalcite catalysts. The role of acid–base pairs pp 140–149

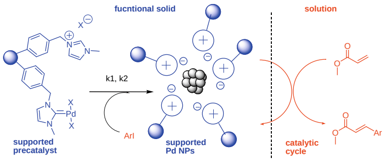
Maria J. Climent, Avelino Corma *, Pilar De Frutos, Sara Iborra, Maria Noy, Alexandra Velty, Patricia Concepción



Glycerol carbonate has been prepared by two different routes using heterogeneous catalysts: transesterification of glycerol with ethylencarbonate and carbonylation of glycerol with urea. Transesterification route using strong Lewis basic catalyst yields high selectivity to glycerol carbonate, while for carbonylation reaction, a catalyst with well balanced acid–base pairs strength is required in order to achieve high selectivity.

Pd catalysts immobilized onto gel-supported ionic liquid-like phases (*g*-SILLPs): A remarkable effect of the nature of the support pp 150–160

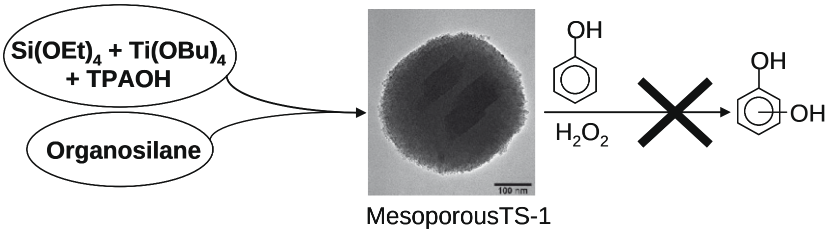
M. Isabel Burguete, Eduardo García-Verdugo *, Ignacio Garcia-Villar, Fabien Gelat, Peter Licence, Santiago V. Luis *, Victor Sans



Catalysis by Pd species supported on *g*-SILLPs of the Heck reaction takes place through a release and catch mechanism allowing an efficient reuse of the resulting heterogeneous systems.

Synthesis and catalytic properties of TS-1 with mesoporous/microporous hierarchical structures obtained in the presence of amphiphilic organosilanes pp 161–168

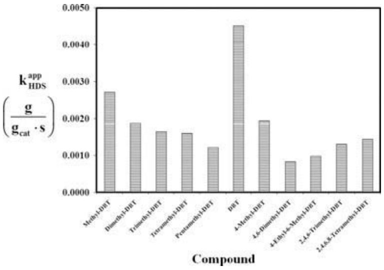
Yohan Cheneviere, Frédéric Chieux, Valérie Caps, Alain Tuel *



The creation of intra-crystalline mesopores in TS-1 does not necessarily improve the activity of the catalyst in phenol hydroxylation.

Kinetic study and H_2S effect on refractory DBTs desulfurization in a heavy gasoil pp 169–178

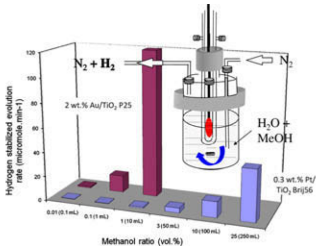
Leonidas E. Kallinikos, Andreas Jess, Nikos G. Papayannakos *



Apparent reaction rate constants of DBTs groups and DBTs individual compounds. Obtained for LHSV: 1–3 h^{-1}, temperature: 613 K, hydrogen pressure: 50×10^5 Pa and gas to liquid ratio: 400 Nm^3/m^3.

Solar light photocatalytic hydrogen production from water over Pt and Au/TiO_2(anatase/rutile) photocatalysts: Influence of noble metal and porogen promotion pp 179–190

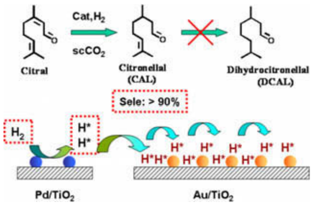
Olivier Rosseler, Muthukonda V. Shankar, Maithaa Karkmaz-Le Du, Loïc Schmidlin, Nicolas Keller *, Valérie Keller



Solar light photocatalytic hydrogen production was obtained from water using low amounts of methanol co-reactant over Pt and Au/TiO_2 (anatase/rutile) photocatalysts, showing the influence of noble metal and porogen promotion.

Physically and chemically mixed TiO_2-supported Pd and Au catalysts: unexpected synergistic effects on selective hydrogenation of citral in supercritical CO_2 pp 191–200

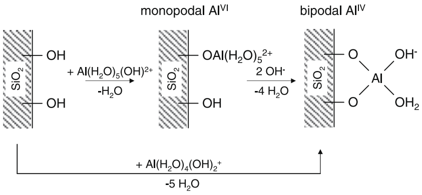
Ruixia Liu, Yancun Yu, Kazuki Yoshida, Guiming Li, Haoxi Jiang, Minhua Zhang, Fengyu Zhao *, Shin-ichiro Fujita, Masahiko Arai *



The synergistic effects between Pd and Au or TiO_2 make the chemically and physically mixed Pd/TO_2 and Au/TiO_2 present unexpected high reaction rate and selectivity in citral hydrogenation in $scCO_2$.

Formation of acid sites in amorphous silica-alumina pp 201–218

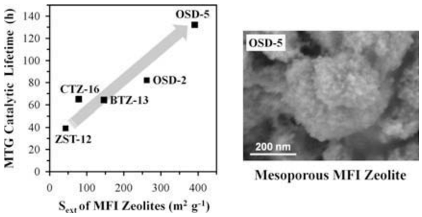
E.J.M. Hensen *, D.G. Poduval, P.C.M.M. Magusin, A.E. Coumans, J.A.R. van Veen



Well-defined precursors to amorphous silica-alumina are prepared through the grafting of aluminium to silica via hydrolytic adsorption. Calcination results in two competing processes, namely the diffusion of aluminium into the silica network to give the desired Brønsted acidity and the surface aggregation into small domains of aluminium oxide.

Effect of mesoporosity against the deactivation of MFI zeolite catalyst during the methanol-to-hydrocarbon conversion process pp 219–228

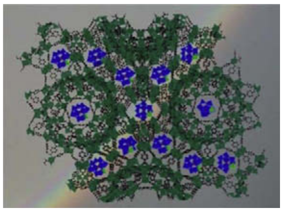
Jeongnam Kim, Minkee Choi, Ryong Ryoo *



Catalytic lifetime of MFI zeolites in methanol-to-hydrocarbon conversion is remarkably improved by mesopore generation. This is attributed to a shift of the location of coke from micropores to mesopore walls.

Building MOF bottles around phosphotungstic acid ships: One-pot synthesis of bi-functional polyoxometalate-MIL-101 catalysts pp 229–241

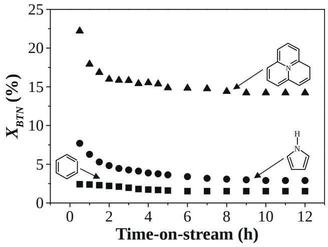
Jana Juan-Alcañiz, Enrique V. Ramos-Fernandez, Ugo Lafont, Jorge Gascon *, Freek Kapteijn



By direct, one-pot, encapsulation of polyoxometalates into MIL-101(Cr), bi-functional porous solids with outstanding catalytic performance in base- and acid-catalyzed reactions are obtained.

Impact of nitrogen doping of carbon nanospheres on the nickel-catalyzed hydrogenation of butyronitrile pp 242–251

Antonio Nieto-Márquez, Diana Toledano, Paula Sánchez, Amaya Romero, José Luis Valverde *



Our results demonstrate that doping carbon nanospheres with nitrogen strongly impacts on reactant adsorption and supported metal sintering, both critical aspects in the hydrogenation of nitriles. Enhanced catalytic activity linked to nitrogen doping was further accused when nitrogen was incorporated in the quaternary form.