



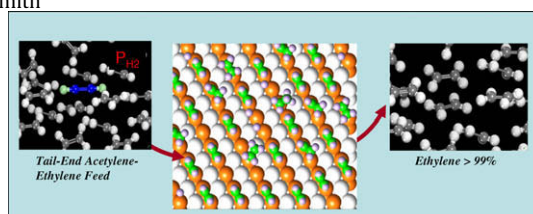
Journal of Catalysis Vol. 268, Issue 2, 2009

Contents

REGULAR ARTICLES

Hydrogenation of acetylene–ethylene mixtures over Pd and Pd–Ag alloys: First-principles-based kinetic Monte Carlo simulations pp 181–195

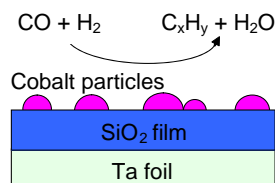
Donghai Mei, Matthew Neurock*, C. Michael Smith



An ab initio kinetic Monte Carlo simulation was constructed to follow the kinetics and the molecular transformation involved in the selective hydrogenation of acetylene from acetylene/ethylene feeds to ethylene over model Pd (1 1 1) and Pd–Ag (1 1 1) alloy surfaces. The simulations reveal that the addition of Ag significantly enhances the selectivity to ethylene by weakening the acetylene-, ethylene-, and hydrogen-bond strength and limits the availability of hydrogen on the surface for reaction. Ethylidyne formation which predominantly occurs on Pd plays a similar role but is less effective.

Fischer–Tropsch synthesis on a model Co/SiO₂ catalyst pp 196–200

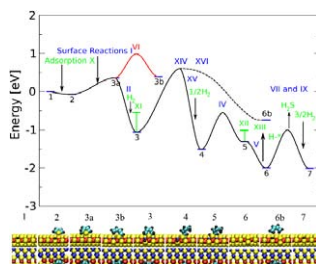
Zhen Yan, Zhoujun Wang, Dragomir B. Bukur, D. Wayne Goodman*



The kinetics and product distributions of Fischer–Tropsch synthesis on a planar model Co/SiO₂ catalyst are in good agreement with those obtained on “real-world” catalysts.

The effect of Co-promotion on MoS₂ catalysts for hydrodesulfurization of thiophene: A density functional study pp 201–208

Poul Georg Moses, Berit Hinnemann*, Henrik Topsøe, Jens K. Nørskov

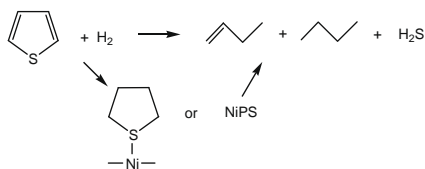


Density functional theory (DFT) calculations of the hydrogenation (HYD) and direct desulfurization (DDS) pathways of thiophene hydrodesulfurization over cobalt-promoted MoS₂. The Co–Mo–S edge is reactive toward both hydrogenation and C–S bond scission.

In situ FTIR and XANES studies of thiophene hydrodesulfurization on Ni₂P/MCM-41

pp 209–222

S. Ted Oyama, Travis Gott, Kiyotaka Asakura*, Satoru Takakusagi, Kotaro Miyazaki, Yuichiro Koike, Kyoko K. Bando*

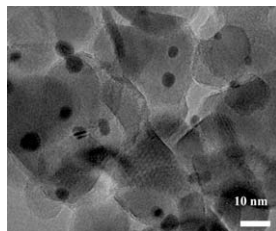


In situ infrared spectroscopy during hydrodesulfurization of thiophene over Ni₂P/MCM-41 showed the presence of tetrahydrothiophene, while transient X-ray absorption spectroscopy showed a Ni–S bond due to this species or a phosphosulfide.

Gold particle size effects in the gas-phase hydrogenation of *m*-dinitrobenzene over Au/TiO₂

pp 223–234

Fernando Cárdenas-Lizana, Santiago Gómez-Quero, Hicham Idriss, Mark A. Keane*

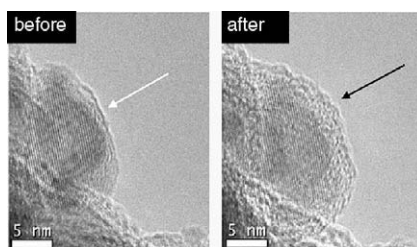


m-Dinitrobenzene hydrogenation over Au/TiO₂ (see TEM image) exhibited a particle size sensitivity delivering higher specific rates over smaller Au particle sizes (in the range 3.4–10.0 nm), irrespective of support anatase:rutile ratio; Au particles <5 nm favour partial –NO₂ reduction to generate *m*-nitroaniline, a response that is linked to Au electronic character, which impacts on *m*-dinitrobenzene adsorption/activation.

Insights into the nature of iron-based Fischer–Tropsch catalysts from quasi in situ TEM-EELS and XRD

pp 235–242

S. Janbroers*, J.N. Louwen, H.W. Zandbergen, P.J. Kooyman



An important issue in iron-based Fischer–Tropsch catalysts is its air-sensitivity. Using both XRD and TEM-EELS in quasi in situ mode, we found that carbon is freed from iron carbides during exposure to air and deposited as a separate amorphous phase. When studying these catalysts, exposure to air should be avoided completely.

Improved 1-butene/isobutane alkylation with acidic ionic liquids and tunable acid/ionic liquid mixtures

pp 243–250

Shengwei Tang, Aaron M. Scurto, Bala Subramaniam*

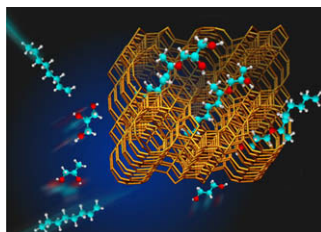


Mixtures of ionic liquids (with acidity manifested in the cation and/or anion) and conventional acids display tunable synergy and offer superior conversion, selectivity, and catalyst stability for the title reaction.

Synthesis of long alkyl chain ethers through direct etherification of biomass-based alcohols with 1-octene over heterogeneous acid catalysts

pp 251–259

Agnieszka M. Ruppert, Andrei N. Parvulescu, Maria Arias, Peter J.C. Hausoul, Pieter C.A. Bruijninx, Robertus J.M. Klein Gebbink, Bert M. Weckhuysen*

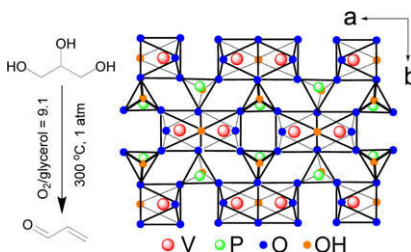


Direct etherification of biomass-based alcohols with 1-octene can be performed over solid acid catalysts such as zeolite Beta as a new route for synthesis of the valuable long alkyl chain ethers with very high selectivities.

Catalytic dehydration of glycerol over vanadium phosphate oxides in the presence of molecular oxygen

pp 260–267

Feng Wang*, Jean-Luc Dubois, Wataru Ueda*

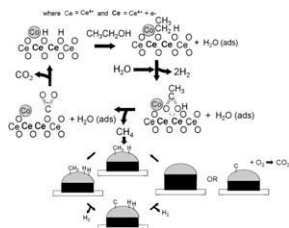


Catalysts of vanadium phosphate oxides were studied in glycerol dehydration to acrolein in the temperature range of 250–350 °C with an O₂/glycerol ratio of 0–13.6.

Study of catalyst deactivation and reaction mechanism of steam reforming, partial oxidation, and oxidative steam reforming of ethanol over Co/CeO₂ catalyst

pp 268–281

Sania M. de Lima, Adriana M. da Silva, Lídia O.O. da Costa, Uschi M. Graham, Gary Jacobs, Burtron H. Davis, Lisiane V. Mattos, Fábio B. Noronha*

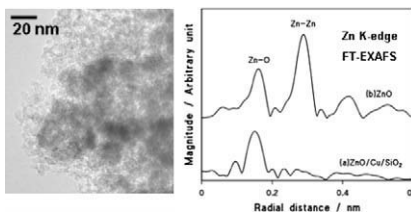


A reaction mechanism was proposed based on in situ DRIFTS and ethanol TPD. Reaction type, feed ratio, and temperature influence amounts and types of carbon deposited and in turn, catalyst stability.

Suppression of CO by-production in steam reforming of methanol by addition of zinc oxide to silica-supported copper catalyst

pp 282–289

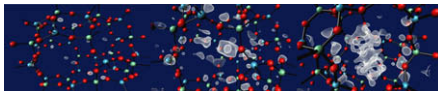
Yasuyuki Matsumura*, Hideomi Ishibe



By-production of CO in methanol steam reforming to H₂ and CO₂ is significantly suppressed by the addition of ZnO to Cu/SiO₂ prepared by a sol-gel method. ZnO is highly dispersed in the catalyst.

SAPO-34 methanol-to-olefin catalysts under working conditions: A combined *in situ* powder X-ray diffraction, mass spectrometry and Raman study pp 290–296

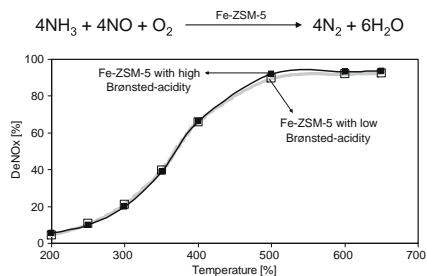
David S. Wragg*, Rune E. Johnsen, Murugan Balasundaram, Poul Norby, Helmer Fjellvåg, Arne Grønvd, Terje Fuglerud, Jasmina Hafizovic, Ørnulv B. Vistad, Duncan Akporiaye



In situ X-ray diffraction and Raman investigations of SAPO-34 during methanol-to-olefin conversion show asymmetric expansion of the catalyst linked to the build-up of intermediates in the zeolite cages.

The role of Brønsted acidity in the selective catalytic reduction of NO with ammonia over Fe-ZSM-5 pp 297–306

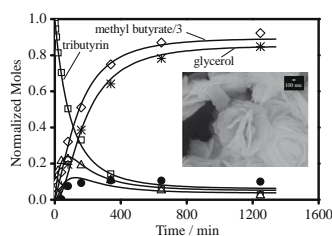
Sandro Brandenberger, Oliver Kröcher*, Alexander Wokaun, Arno Tessler, Roderik Althoff



The selective catalytic reduction of NO with NH₃ has been studied over Fe-ZSM-5 samples with equal exchange degrees and active sites but different Brønsted-acidities. The experiments revealed that the acidity of the catalyst is not a crucial factor for high activity and that Brønsted-acidity may not be required for adsorbing or activating the ammonia.

Influence of textural properties and trace water on the reactivity and deactivation of reconstructed layered hydroxide catalysts for transesterification of tributyrin with methanol pp 307–317

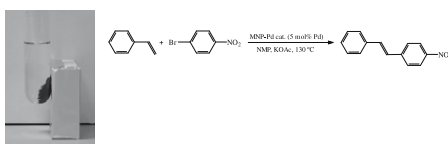
Yuanzhou Xi, Robert J. Davis*



Variations in the textural properties of reconstructed hydrotalcites did not significantly affect the surface base site density or turnover rate of tributyrin transesterification with methanol. However, trace water enhanced the rate of transesterification and promoted severe catalyst deactivation by hydrolysis.

Easy-separable magnetic nanoparticle-supported Pd catalysts: Kinetics, stability and catalyst re-use pp 318–328

Urszula Laska, Christopher G. Frost, Gareth J. Price, Pawel K. Plucinski*

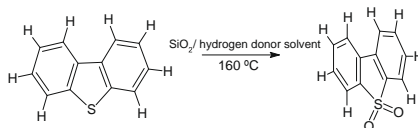


The kinetics of C–C coupling reactions and hydrogenation were studied to investigate the reactivity and separation effectiveness of palladium-based magnetic nanocatalysts.

Oxidation of dibenzothiophene to dibenzothiophene-sulfone using silica gel

pp 329–334

Karina Castillo*, J.G. Parsons, David Chavez, Russell R. Chianelli

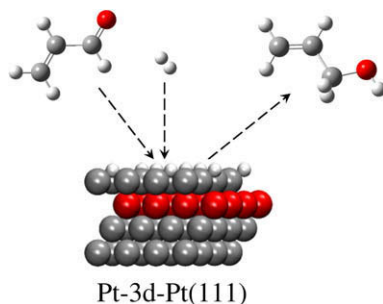


We present a process for oxidizing dibenzothiophene (DBT) to dibenzothiophene-sulfone (DBT-sulfone) using silica gel in the presence of a hydrogen donor solvent where no oxidizing agent was necessary.

Trend in the C=C and C=O bond hydrogenation of acrolein on Pt–M (M = Ni, Co, Cu) bimetallic surfaces

pp 335–342

Luis E. Murillo, Carl A. Menning, Jingguang G. Chen*

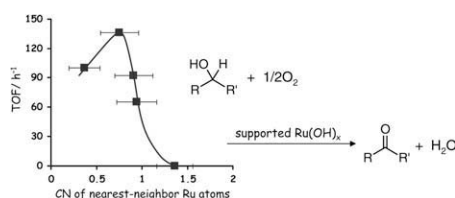


Pt-3d-Pt(1 1 1) structures, where 3d = Ni or Co, are shown to have increased activity for the selective hydrogenation of the C=O bond of acrolein.

Aerobic alcohol oxidation catalyzed by supported ruthenium hydroxides

pp 343–349

Kazuya Yamaguchi, Jung Won Kim, Jinling He, Noritaka Mizuno*

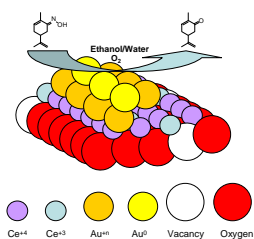


The supported Ru(OH)_x catalysts could act as efficient heterogeneous catalysts for the aerobic oxidation alcohols. The present oxidation was dependent on the coordination number of nearest-neighbor Ru atoms.

Gold nanoparticles supported on ceria promote the selective oxidation of oximes into the corresponding carbonylic compounds

pp 350–355

Abdessamad Grirrane, Avelino Corma*, Hermenegildo Garcia*

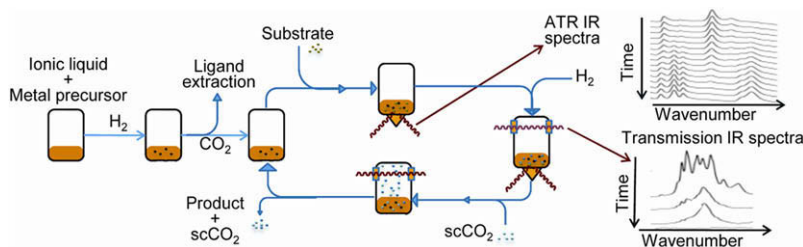


Aliphatic and aromatic oximes, including carboxime, can be converted into the corresponding ketones and aldehydes using oxygen as a reagent and gold nanoparticles supported on nanoparticulated ceria as catalysts.

A green pathway for hydrogenations on ionic liquid-stabilized nanoparticles

pp 356–366

Fabian Jutz, Jean-Michel Andanson, Alfons Baiker*

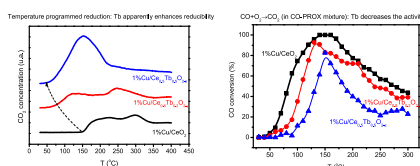


Palladium and Rhodium nanoparticles were synthesized in different ionic liquids and subsequently used as catalysts in solventless hydrogenations. Supercritical carbon dioxide served for the removal of metal precursor ligands and product extraction.

CO-TPR-DRIFTS-MS *in situ* study of CuO/Ce_{1-x}Tb_xO_{2-y} (x = 0, 0.2 and 0.5) catalysts: Support effects on redox properties and CO oxidation catalysis

pp 367–375

Aitor Hornés, Parthasarathi Bera, Antonio López Cámara, Daniel Gamarra, Guillermo Munuera, Arturo Martínez-Arias*

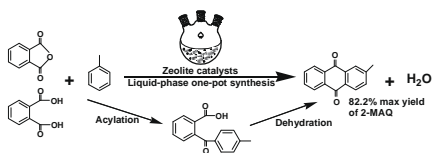


Reasons for the discrepancies between redox and catalytic properties on the basis of classical CO temperature-programmed reduction tests starting at room temperature are explored in Ce_{1-x}Tb_xO_{2-y}-supported copper catalysts by *in situ* infrared.

Liquid-phase cascade acylation/dehydration over various zeolite catalysts to synthesize 2-methylantraquinone through an efficient one-pot strategy

pp 376–383

Qijun Hou, Bumei Zheng, Chenguang Bi, Jimei Luan, Zhongkui Zhao*, Hongchen Guo, Guiru Wang, Zongshi Li



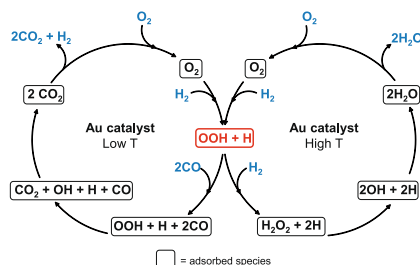
Liquid-phase cascade acylation/dehydration promoted by H-beta zeolite is an effectual strategy to yield 2-methylantraquinone in 82.2%. The acidity and morphology strongly affect catalytic properties and coke formation.

RESEARCH NOTE

On the mechanism of hydrogen-promoted gold-catalyzed CO oxidation

pp 384–389

Elodie Quinet, Laurent Piccolo*, Franck Morfin, Priscilla Avenier, Fabrice Diehl, Valérie Caps, Jean-Luc Rousset



H₂ promotes low-temperature CO oxidation on gold via the formation of hydroperoxy intermediates, also present in hydrogen oxidation.