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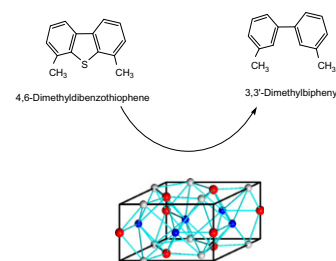
Contents

PRIORITY COMMUNICATION

Unprecedented selectivity to the direct desulfurization (DDS) pathway in a highly active FeNi bimetallic phosphide catalyst

pp 1–5

S. Ted Oyama*, Haiyan Zhao, Hans-Joachim Freund, Kiyotaka Asakura, Radosław Włodarczyk, Marek Sierka



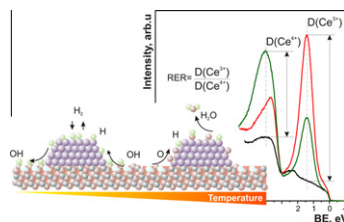
A bimetallic NiFe phosphide catalyst shows high selectivity for the deep hydrodesulfurization of 4,6-dimethylbenzothiophene to diphenyl.

REGULAR ARTICLES

Hydrogen spillover monitored by resonant photoemission spectroscopy

pp 6–9

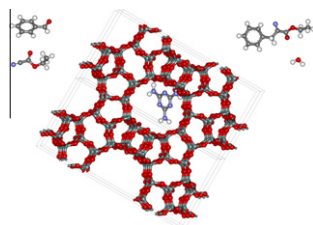
Yaroslava Lykhach*, Thorsten Staudt, Mykhailo Vorokhta, Tomáš Skála, Viktor Johánek, Kevin C. Prince, Vladimír Matolín, Jörg Libuda

Hydrogen spillover, a critical mechanistic step on nanostructured ceria catalysts, gives rise to reversible changes of the oxidation state of surface cerium ions. Applying resonant photoemission spectroscopy to Pt/CeO₂ model catalyst, these changes are monitored with highest sensitivity, thus providing detailed mechanistic insight into surface hydrogen migration.

A designed organic–zeolite hybrid acid–base catalyst

pp 10–18

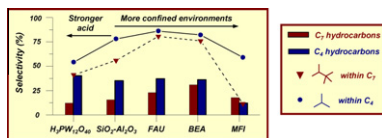
Andrew C. Brooks, Liam France, Cecile Gayot, Jerry Pui Ho Li, Ryan Sault, Andrew Stafford, John D. Wallis, Michael Stockenhuber*

Benzaldehyde and ethylcyanoacetate react over a zeolite modified with melamine to form trans- α -cyanocinnamate.

Acid strength and solvation effects on methylation, hydride transfer, and isomerization rates during catalytic homologation of C₁ species

pp 19–30

Dante A. Simonetti, Robert T. Carr, Enrique Iglesia*

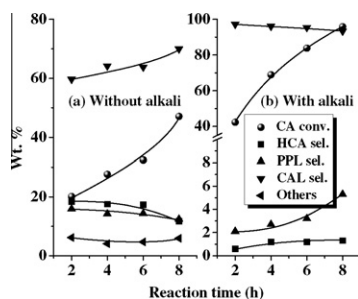


Formation of isobutane and triptane from C₁ precursors is favored on all solid acids, because methylation and hydride transfer steps selectively grow hydrocarbons without significant deviations via isomerization steps. Triptane and isobutane selectivities are maximized on BEA and FAU because weak acid sites and confinement within large channels preferentially stabilize hydride transfer and methylation transition states that preserve the structure of triptane in growing hydrocarbons over isomerization transition states.

Intramolecular selective hydrogenation of cinnamaldehyde over CeO₂–ZrO₂-supported Pt catalysts

pp 31–40

S. Bhogeswararao, D. Srinivas*

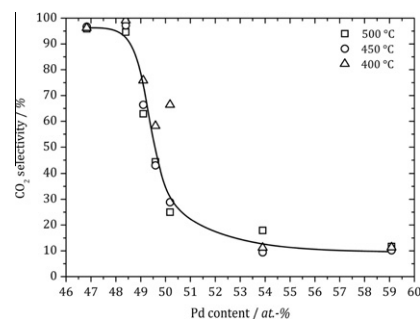


Selective liquid phase hydrogenation of cinnamaldehyde is reported, for the first time, over CeO₂–ZrO₂-supported Pt catalysts, which are highly active and selective even at 25 °C.

Influence of bulk composition of the intermetallic compound ZnPd on surface composition and methanol steam reforming properties

pp 41–47

Matthias Friedrich, Detre Teschner, Axel Knop-Gericke, Marc Armbrüster*

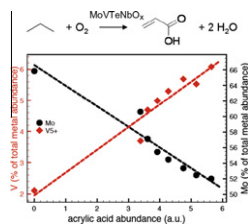


Methanol steam reforming was studied on unsupported ZnPd intermetallic compounds with different compositions proving Zn-rich compounds to show excellent CO₂ selectivity compared to Pd-rich compounds.

Surface chemistry of phase-pure M1 MoVTeNb oxide during operation in selective oxidation of propane to acrylic acid

pp 48–60

Michael Hävecker, Sabine Wrabetz, Jutta Kröhnert, Lenard-Istvan Csepei, Raoul Naumann d'Alnoncourt, Yury V. Kolen'ko, Frank Girgsdies, Robert Schlögl, Annette Trunschke*

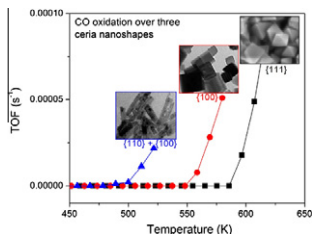


The surface of a highly crystalline MoVTeNb oxide catalyst composed exclusively of the M1 phase has been studied before catalysis and during operation in oxidation of propane at 693 K. Increasing formation of acrylic acid in general goes along with surface depletion of Mo and accordingly the enrichment in Te, V, and Nb. A close correlation exists between the acrylic acid production and the increasing presence of surface V⁵⁺ species.

On the structure dependence of CO oxidation over CeO₂ nanocrystals with well-defined surface planes

pp 61–73

Zili Wu*, Meijun Li, Steven H. Overbury*

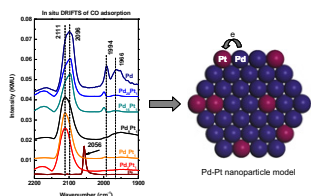


Not only the interaction between CO and ceria but also the reactivity and mobility of lattice oxygen in ceria are greatly influenced by the surface structure of ceria, leading to the strong variation in CO oxidation over ceria nanoshapes.

Pt promotional effects on Pd–Pt alloy catalysts for hydrogen peroxide synthesis directly from hydrogen and oxygen

pp 74–82

Jing Xu, Like Ouyang, Guo-Jin Da, Qian-Qian Song, Xue-Jing Yang, Yi-Fan Han*

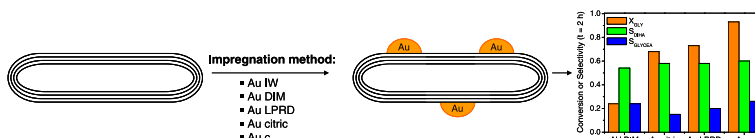


H₂O₂ synthesis directly from H₂ and O₂ over supported Pd–Pt alloy catalysts was studied using a tri-phase reactor under ambient conditions. Pd₁₆Pt₁ showed the best performance with a rate of 1.77 mol h⁻¹ g_{Pd}⁻¹ and a selectivity of 60% while 0.99 mol h⁻¹ g_{Pd}⁻¹ and only 12% observed for pure Pd.

Gold supported on carbon nanotubes for the selective oxidation of glycerol

pp 83–91

Elodie G. Rodrigues, Sónia A.C. Carabineiro, Juan J. Delgado, X. Chen, Manuel F.R. Pereira, José J.M. Órfão*

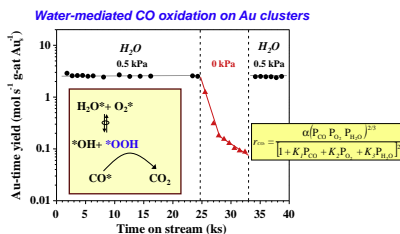


A remarkable high selectivity to dihydroxyacetone combined with a high activity is obtained in the glycerol oxidation over Au/MWCNT catalysts, particularly if the sol immobilization technique is used for the impregnation of gold.

Mechanistic interpretation of CO oxidation turnover rates on supported Au clusters

pp 92–102

Manuel Ojeda, Bi-Zeng Zhan, Enrique Iglesia*

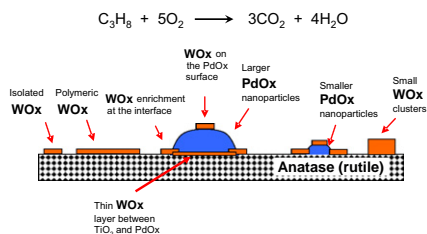


Kinetic and isotopic data show that H₂O acts as a co-catalyst for the activation of O₂ and the retention of catalytic reactivity in CO oxidation on Au clusters. H₂O mediates O₂ activation steps, circumvents the kinetic bottlenecks prevalent under anhydrous conditions, and accounts for the remarkable reactivity of monofunctional Au metal clusters at near ambient temperatures.

Synergy between tungsten and palladium supported on titania for the catalytic total oxidation of propane

pp 103–114

Marie N. Taylor, Wu Zhou, Tomas Garcia*, Benjamin Solsona, Albert F. Carley, Christopher J. Kiely, Stuart H. Taylor*

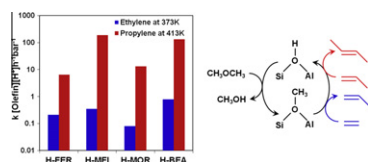


Titania-supported palladium catalysts modified by the addition of tungsten were studied for the total oxidation of propane. The addition of tungsten significantly improved catalyst performance, and this is related to the structure of the catalyst.

Kinetics and mechanism of olefin methylation reactions on zeolites

pp 115–123

Ian M. Hill, Saleh Al Hashimi, Aditya Bhan*

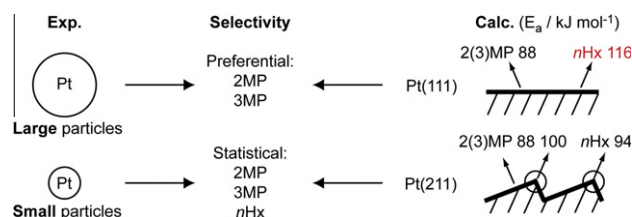


Dimethyl ether methylation of olefins proceeds via the same mechanistic pathway on different zeolites, but with different rates of reaction showing that zeolites propagate olefin methylation reaction cycles prevalent in methanol-to-hydrocarbons conversion to varying extents. The formation and involvement of surface methoxide species is consistent with the secondary kinetic isotope effect observed using CD₃OCD₃ reactants and with olefin methylation rates having a zero-order dependence in DME pressures and a first-order dependence in olefin pressure.

Tuning the selectivity for ring-opening reactions of methylcyclopentane over Pt catalysts: A mechanistic study from first-principles calculations

pp 124–133

Zhi-jian Zhao, Lyudmila V. Moskaleva, Notker Rösch*

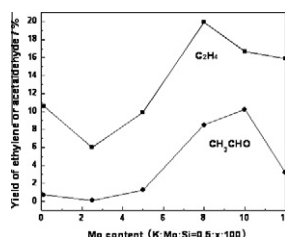


Methylcyclopentane is a benchmark model system to study selective ring-opening of hydrocarbons on supported Pt. Electronic structure calculations show that the distribution of possible ring-opening products, *n*-hexane (*n*Hx) and its branched isomers, 2- and 3-methylpentane (2MP and 3MP), is controlled by the height of the C–C bond scission barrier.

Potassium-modified molybdenum-containing SBA-15 catalysts for highly efficient production of acetaldehyde and ethylene by the selective oxidation of ethane

pp 134–144

Jian Liu, Lihong Yu, Zhen Zhao*, Yongsheng Chen*, Pengyu Zhu, Chao Wang, Yan Luo, Chunming Xu, Aijun Duan, Guiyuan Jiang

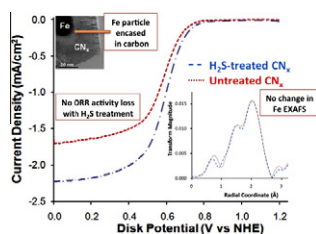


Potassium-modified K/Mo-SBA-15 catalysts give supercatalytic performance for the selective oxidation of ethane to acetaldehyde and ethylene. The maximum yields of acetaldehyde and ethylene can reach 10.2% and 19.9%, respectively.

Investigation of sulfur poisoning of CN_x oxygen reduction catalysts for PEM fuel cells

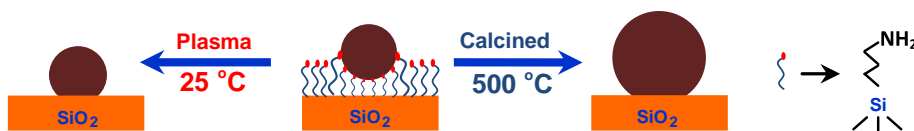
pp 145–151

Dieter von Deak, Deepika Singh, Elizabeth J. Biddinger, Jesaiah C. King, Burcu Bayram, Jeffrey T. Miller, Umit S. Ozkan*

Examining the role of Fe in CN_x materials for oxygen reduction reaction by deliberate poisoning with H₂S.**Room temperature O₂ plasma treatment of SiO₂ supported Au catalysts for selective hydrogenation of acetylene in the presence of large excess of ethylene**

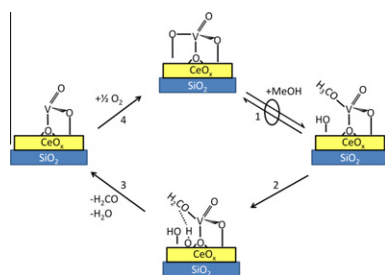
pp 152–159

Xiaoyan Liu, Chung-Yuan Mou*, Szetsen Lee, Yanan Li, Jeremiah Secrest, Ben W.-L. Jang*

The O₂ plasma working under mild conditions can remove the organic compounds efficiently without causing aggregation of gold nanoparticles. The O₂ plasma-treated Au/SiO₂ showed good catalytic performances in the selective hydrogenation of C₂H₂ in large excess of C₂H₄ at low temperature, which might be due to the small size and the nearly neutral charge of gold nanoparticles.**Investigation of the structure and activity of VO_x/CeO₂/SiO₂ catalysts for methanol oxidation to formaldehyde**

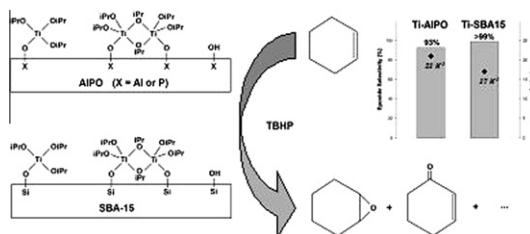
pp 160–167

William C. Vining, Jennifer Strunk, Alexis T. Bell*

An investigation of methanol oxidation to formaldehyde was carried out using bilayered VO_x/CeO₂/SiO₂ catalysts consisting of pseudo-tetrahedral vanadate species supported on an amorphous ceria layer. The activity of VO_x/CeO₂/SiO₂ was about 20-fold higher than that of VO_x/SiO₂. This difference is attributed to the differences in the rate-limiting step for formaldehyde formation on the two catalysts.**Epoxidation catalysts derived from introduction of titanium centers onto the surface of mesoporous aluminophosphate: Comparisons with analogous catalysts based on mesoporous silica**

pp 168–176

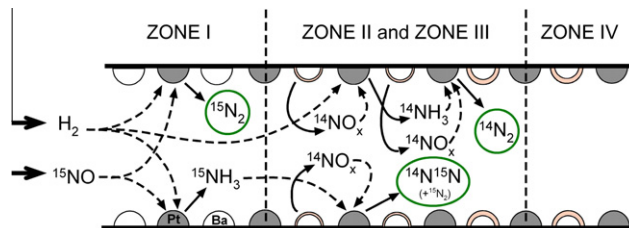
Lorraine Raboin, Junko Yano, T. Don Tilley*



Mesoporous aluminophosphates were grafted by titanium isopropoxide and investigated as catalysts for the oxidation of cyclohexene. The Ti-AIPO catalysts have comparable structural and catalytic properties than similar Ti-SBA15 catalysts, but exhibit a higher tendency toward allylic oxidation.

Regeneration mechanism of a Lean NO_x Trap (LNT) catalyst in the presence of NO investigated using isotope labelling techniques pp 177–186

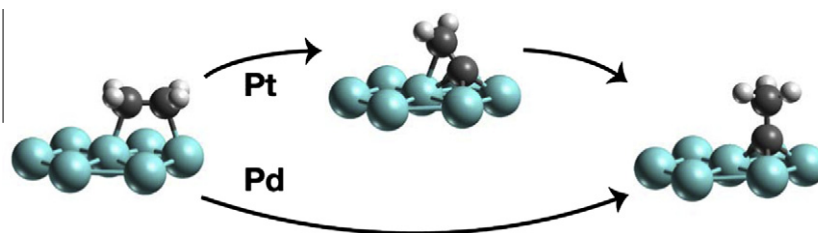
Beñat Pereda-Ayo*, Juan R. González-Velasco, Robbie Burch, Christopher Hardacre, Sarayute Chansai*



The evolution of products formed from reduction of stored nitrates on a Pt–Ba/Al₂O₃ LNT catalyst is significantly modified by the presence of NO during the regeneration. Isotope labelling techniques allowed us to propose three different routes for N₂/NH₃ formation; extension of which is affected by the H₂ concentration.

Ethylene conversion to ethylidyne on Pd(1 1 1) and Pt(1 1 1): A first-principles-based kinetic Monte Carlo study pp 187–195

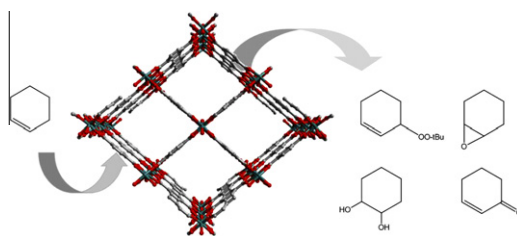
Hristiyan A. Aleksandrov, Lyudmila V. Moskaleva, Zhi-Jian Zhao, Duygu Basaran, Zhao-Xu Chen, Donghai Mei*, Notker Rösch*



kMC Simulations predict that the most plausible pathway on the Pd(1 1 1) and Pt(1 1 1) surfaces is ethylene → vinyl → vinylidene → ethylidyne.

The coordinatively saturated vanadium MIL-47 as a low leaching heterogeneous catalyst in the oxidation of cyclohexene pp 196–207

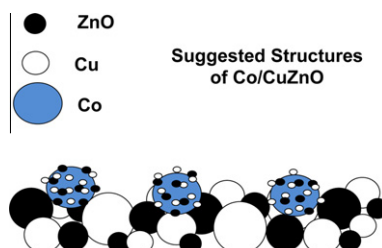
Karen Leus, Matthias Vandichel, Ying-Ya Liu, Ilke Muylaert, Jan Musschoot, Steven Pyl, Henk Vrielinck, Freddy Callens, Guy B. Marin, Christophe Detavernier, Paul V. Wiper, Yaroslav Z. Khimyak, Michel Waroquier, Veronique Van Speybroeck*, Pascal Van Der Voort*



V-MIL-47 is evaluated as a catalyst in the epoxidation of cyclohexene. Experimental results, combined with computational modelling confirm that at least two parallel catalytic cycles are co-existing: one with V+IV sites and one with pre-oxidized V+V sites.

Effect of component interaction on the activity of Co/CuZnO for CO hydrogenation pp 208–215

Xunhua Mo, Yu-Tung Tsai, Jia Gao, Dongsen Mao, James G. Goodwin Jr.*

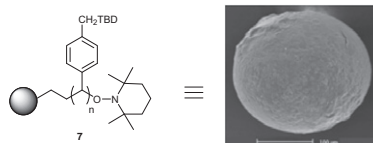


ZnO and Cu decorate the Co surface, blocking a substantial number of active sites on Co for CO hydrogenation.

Rasta resin as support for TBD in base-catalyzed organic processes

pp 216–222

Simona Bonollo, Daniela Lanari*, Tommaso Angelini, Ferdinando Pizzo, Assunta Marrocchi, Luigi Vaccaro*

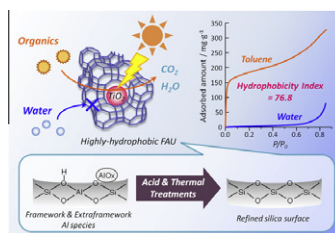


In this contribution Rasta polymer has been used to preparation of high-loading Rasta-TBD. This catalyst has been able to efficiently promote several organic transformations with constantly good and promising results.

TiO₂ photocatalyst for degradation of organic compounds in water and air supported on highly hydrophobic FAU zeolite: Structural, sorptive, and photocatalytic studies

pp 223–234

Yasutaka Kuwahara, Junya Aoyama, Keisuke Miyakubo, Taro Eguchi, Takashi Kamegawa, Kohsuke Mori, Hiromi Yamashita*

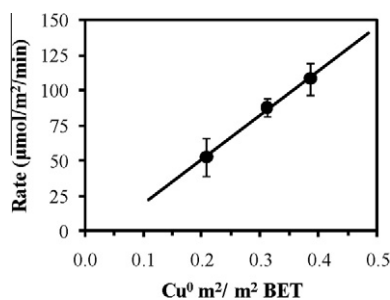


Faujasite zeolite of high crystallinity, stability, and hydrophobicity improves the photocatalytic degradation of 2-propanol in water and acetaldehyde in air when used as catalyst support for TiO₂.

Active species of copper chromite catalyst in C–O hydrogenolysis of 5-methylfurfuryl alcohol

pp 235–241

Keenan L. Deusch, Brent H. Shanks*

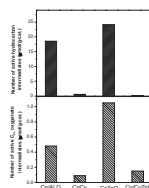


The roles of the Cu⁰ and Cu⁺ species in a copper chromite catalyst, CuCr₂O₄·CuO, in the condensed-phase hydrogenolysis of 5-methylfurfuryl alcohol to 2,5-dimethylfuran were investigated. The maxima of both active species occurred after reduction at 300 °C for 1 h. The correlation between Cu⁰ and specific activity suggested that Cu⁰ was primarily responsible for catalytic activity.

The synthesis of hydrocarbons and oxygenates during CO hydrogenation on CoCuZnO catalysts: Analysis at the site level using multiproduct SSITKA

pp 242–250

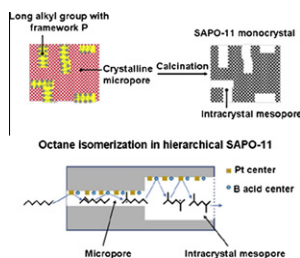
Yu-Tung Tsai, Xunhua Mo, James G. Goodwin Jr.*



Compared to Co/Al₂O₃, the addition of Cu to Co decreases the concentrations of active surface intermediates significantly for both hydrocarbons and C₂₊ oxygenates while those quantities can increase somewhat with ZnO. The high selectivities for C₂₊ oxygenates observed for Co/CuZnO are due to the low concentration of active surface intermediates for hydrocarbons relative to that for oxygenates.

Alkylphosphonic acid- and small amine-templated synthesis of hierarchical silicoaluminophosphate molecular sieves with high isomerization selectivity to di-branched paraffins pp 251–259

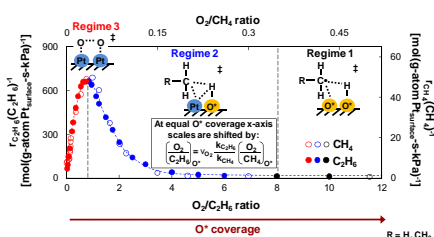
Yu Fan, Han Xiao, Gang Shi, Haiyan Liu, Xiaojun Bao*



The P atoms in alkylphosphonic acid are introduced into the SAPO-11 framework, and thus the long alkyl groups bonded with these P atoms induce the formation of intracrystal mesopores after calcination. The interpenetrating micro-mesoporous channels of the hierarchical SAPO-11 endow the resulting catalyst with the superior di-branched isomer selectivity.

Catalytic reactions of dioxygen with ethane and methane on platinum clusters: Mechanistic connections, site requirements, and consequences of chemisorbed oxygen pp 260–272

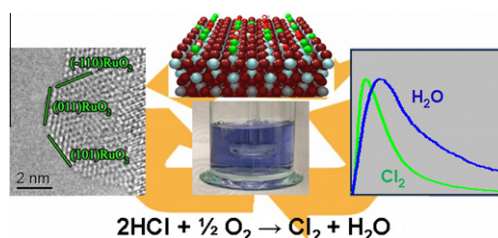
Mónica García-Diéguez, Ya-Huei (Cathy) Chin, Enrique Iglesia*



Kinetic and isotopic data and Pt cluster size effects show that $C_2H_6-O_2$ and CH_4-O_2 form CO_2 and H_2O via analogous elementary steps; turnover rates are higher for C_2H_6 in all kinetic regimes where C–H bond cleavage limits rates because weaker C–H bonds in C_2H_6 and stronger ethyl interactions with adsorbed oxygens (O^*) at transition states lead to lower barriers for C_2H_6 than for CH_4 activation. Reactivity differences cause transitions between kinetic regimes to occur at higher O_2 /alkane ratios for C_2H_6 because it scavenges O^* species more effectively than CH_4 and leads to lower O^* coverages. These mechanistic analogies and insights can be rigorously extended to other alkanes and metal clusters.

An integrated approach to Deacon chemistry on RuO₂-based catalysts pp 273–284

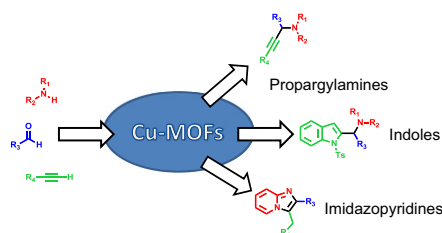
Detre Teschner*, Ramzi Farra, Lide Yao, Robert Schlögl, Hary Soerijanto, Reinhard Schomäcker, Timm Schmidt, László Szentmiklósi, Amol P. Amrute, Cecilia Mondelli, Javier Pérez-Ramírez, Gerard Novell-Leruth, Núria López*



By using state-of-the-art experiments and theoretical calculations, we unravel mechanistic details of HCl oxidation on the industrially relevant RuO_2/SnO_2 catalyst. On the extensively chlorinated surface, oxygen activation is the rate determining step.

Bridging homogeneous and heterogeneous catalysis with MOFs: Cu-MOFs as solid catalysts for three-component coupling and cyclization reactions for the synthesis of propargylamines, indoles and imidazopyridines pp 285–291

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

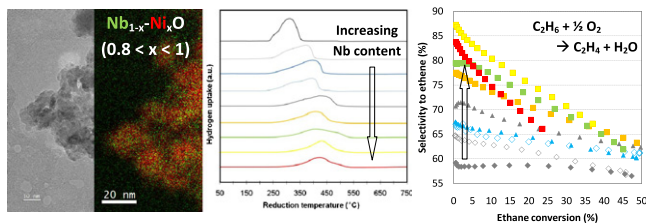


Copper-containing MOFs are highly active catalysts for one-pot three-component coupling reactions of amines, alkynes and aldehydes to form propargylamines. When an additional intramolecular cyclization step is included, indole and imidazopyridines can also be efficiently formed.

Nb effect in the nickel oxide-catalyzed low-temperature oxidative dehydrogenation of ethane

pp 292–303

Haibo Zhu, Samy Ould-Chikh, Dalaver H. Anjum, Miao Sun, Gregory Biousque, Jean-Marie Basset, Valérie Caps*

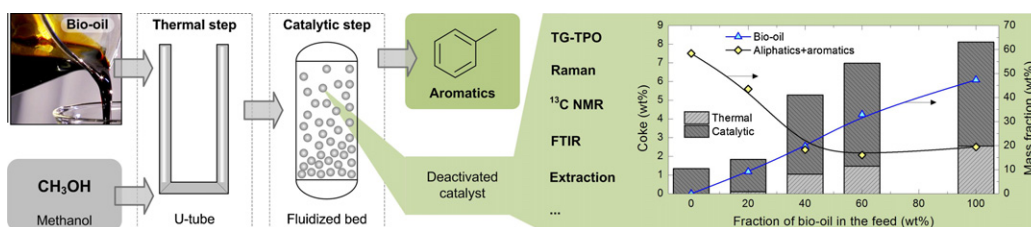


Nb-NiO nanocomposites, which are prepared with a high surface area for the first time, prove highly active for low temperature ethane ODH. Structural and catalytic properties are discussed as a function of the Nb content.

Deactivating species in the transformation of crude bio-oil with methanol into hydrocarbons on a HZSM-5 catalyst

pp 304–314

Beatriz Valle*, Pedro Castaño, Martin Olazar, Javier Bilbao, Ana G. Gayubo

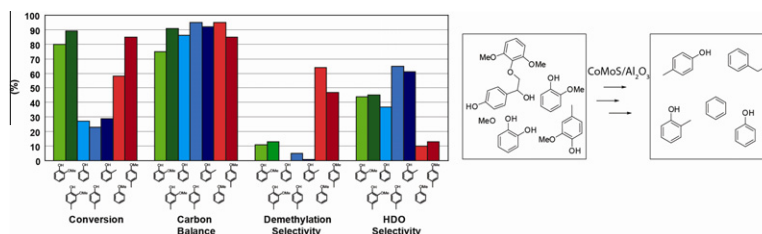


The nature of the coke deposited on a HZSM-5 catalyst (modified with Ni) in the transformation of crude bio-oil was studied. Co-feeding methanol attenuates coke deposition and affects the heterogeneous and oxygenated nature of the coke.

CoMo sulfide-catalyzed hydrodeoxygenation of lignin model compounds: An extended reaction network for the conversion of monomeric and dimeric substrates

pp 315–323

Anna L. Jongorius, Robin Jastrzebski, Pieter C.A. Bruijninx, Bert M. Weckhuysen*



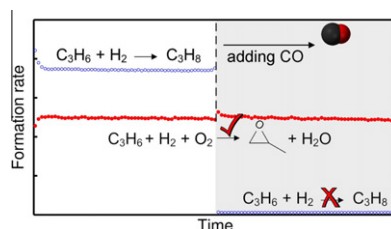
Extensive hydrodeoxygenation studies with a sulfided CoMo/Al₂O₃ catalyst were performed on a library of lignin model compounds. An extended reaction network is proposed, showing that HDO, demethylation, and hydrogenation reactions take place simultaneously.

NOTE

Switching off propene hydrogenation in the direct epoxidation of propene over gold–titania catalysts

pp 324–327

Jiaqi Chen, Sander J.A. Halin, Dulce M. Perez Ferrandez, Jaap C. Schouten, T. Alexander Nijhuis*



Carbon monoxide switches off propene hydrogenation in the direct epoxidation of propene with hydrogen and oxygen over Au/Ti-SiO₂ catalysts.