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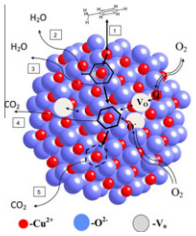
Reaction network for the total oxidation of toluene over $CuO–CeO_2/Al_2O_3$ pp 1–9

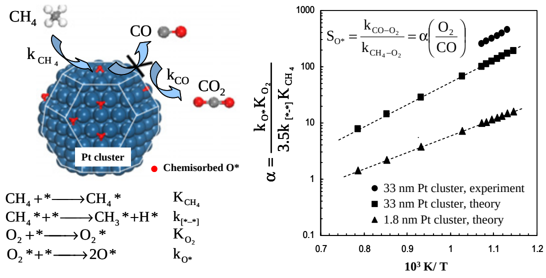
Unmesh Menon, Vladimir V. Galvita*, Guy B. Marin



Alternating pulse and isotopic labeling experiments indicate that the catalytic total oxidation of toluene over $CuO–CeO_2/\gamma-Al_2O_3$ consists of the following sequence: parallel adsorption of toluene on the catalyst surface, step 1; the simultaneous abstraction of H from the methyl and the phenyl group, steps 2 and 3; abstraction of the methyl carbon atom, step 4, followed by destruction of the aromatic ring, step 5. Two types of oxygen are directly involved in the oxidation of toluene: adsorbed oxygen and weakly bound surface lattice oxygen.

Selectivity of chemisorbed oxygen in C–H bond activation and CO oxidation and kinetic consequences for $CH_4–O_2$ catalysis on Pt and Rh clusters pp 10–24

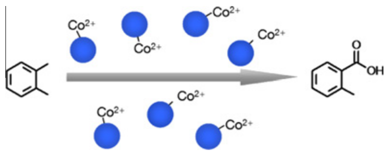
Ya-Huei (Cathy) Chin, Corneliu Buda, Matthew Neurock*, Enrique Iglesia*



Chemisorbed oxygen (O^*) preferentially reacts with CO instead of CH_4 during $CH_4–O_2$ catalysis on Pt and Rh clusters. High O^* selectivities (SO*) for CO reactions with O^* lead to very low CO yields when O_2 is present, indicating that direct catalytic partial oxidation to form CO (and H_2) from $CH_4–O_2$ reactants is unlikely to occur at the molecular scale or at CH_4 conversions of practical interest.

Selective liquid phase oxidation of *o*-xylene with gaseous oxygen by transition metal containing polysiloxane initiator/catalyst systems pp 25–33

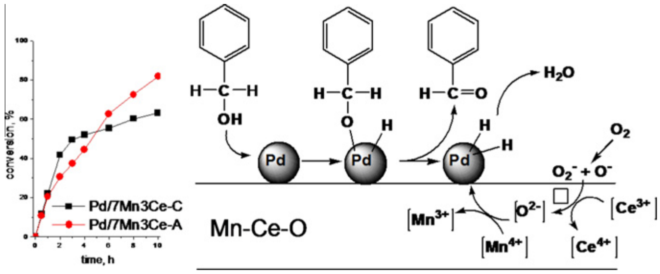
Tobias Förster, Stephan A. Schunk, Andreas Jentys, Johannes A. Lercher*



New solid initiator/catalyst systems (Co^{2+} and Mn^{3+} cation modified hydrophobic polysiloxanes) for the selective liquid phase oxidation are introduced, which show a high stability under reaction conditions and a higher activity than the Co naphthenate benchmark system.

Pd catalysts supported on $MnCeO_x$ mixed oxides and their catalytic application in solvent-free aerobic oxidation of benzyl alcohol: Support composition and structure sensitivity — pp 34–44

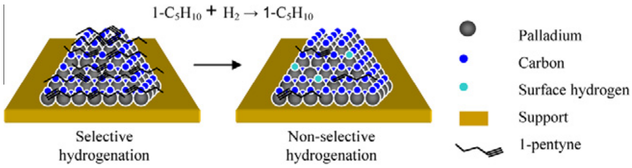
Yuanting Chen, Huijian Zheng, Zhen Guo, Chunmei Zhou, Chuan Wang, Armando Borgna*, Yanhui Yang*



The aerobic oxidation of benzyl alcohol over Pd catalysts supported on crystalline and amorphous $MnCeO_x$ was studied to examine the support composition and structure sensitivity. Pd acts as the sole active species, and the synergetic interactions among Pd, MnO_x, and CeO_2 improve both activity and selectivity.

The roles of carbide and hydride in oxide-supported palladium nanoparticles for alkyne hydrogenation — pp 45–54

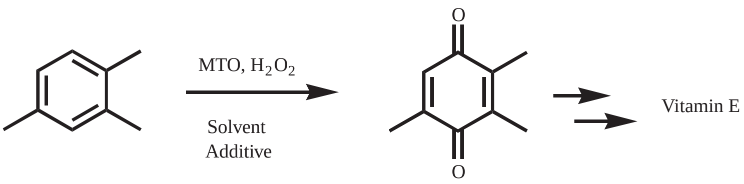
Min Wei Tew, Markus Janousch, Thomas Huthwelker, Jeroen A. van Bokhoven*



Selective and non-selective hydrogenation of 1-pentyne occurs over carbided oxide-supported palladium nanoparticles. Surface poisoning of the palladium carbide-like phase by alkyne is responsible for the constantly high selectivity up to almost 100% conversion. When the reaction became non-selective, the carbide-like structure remained: Full hydrogenation can also occur in the absence of hydride.

Methyltrioxorhenium-catalyzed oxidation of pseudocumene for vitamin E synthesis: A study of solvent and ligand effects — pp 55–67

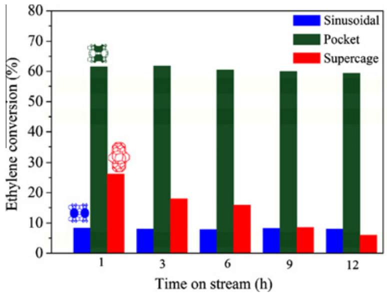
Mónica Carril, Philipp Altmann, Markus Drees, Werner Bonrath, Thomas Netscher, Jan Schütz, Fritz E. Kühn*



The MTO-catalyzed oxidation of pseudocumene for vitamin E synthesis was studied. Solvent and ligand influences were examined to optimize the reaction. Good yields and selectivities were obtained under relatively mild conditions.

Catalytic role of different pore systems in MCM-49 zeolite for liquid alkylation of benzene with ethylene — pp 68–74

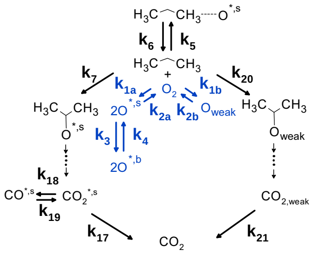
Kefeng Liu, Sujuan Xie, Shenglin Liu, Guoliang Xu, Ningning Gao, Longya Xu*



Surface pockets of MCM-49 are the main place for the liquid alkylation of benzene with ethylene. The generation of heavy aromatics within the supercage system is the main reason for the deactivation of MCM-49 catalyst at the early reaction stage.

Kinetic modeling of the total oxidation of propane over Cu- and Ce-based catalysts pp 75–88

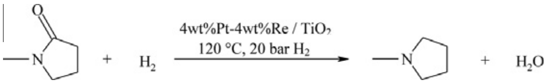
V. Balcaen, H. Poelman*, D. Poelman, G.B. Marin



Propane total oxidation over CuO–CeO$_2$/γ-Al$_2$O$_3$ occurs through a reaction network with kinetically significant steps for reduction, steps 5–7 and 17–21, and re-oxidation, steps 1–4, involving surface lattice oxygen, $O^{*,s}$, and weakly bound oxygen, O_{weak}. Intermediate, kinetically non-significant steps are represented by dots between arrows. The constructed models describe adequately the redox processes, both combined and individually, from 623 K to 873 K.

Catalytic hydrogenation of tertiary amides at low temperatures and pressures using bimetallic Pt/Re-based catalysts pp 89–97

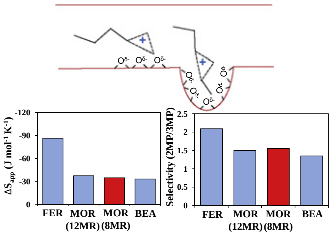
R. Burch, C. Paun, X.-M. Cao, P. Crawford, P. Goodrich, C. Hardacre, P. Hu*, L. McLaughlin, J. Sá, J.M. Thompson*



A bimetallic Pt–Re catalyst can facilitate the hydrogenation of *N*-methylpyrrolidin-2-one to *N*-methylpyrrolidine to high conversion at low temperature and pressure. Catalyst preparation, characterisation and kinetic analysis combined with DFT calculations have shown that the role of rhenium is to activate the carbonyl bond, whilst that of the platinum is as a hydrogenation catalyst, removing intermediates from the surface of the catalyst.

Catalytic consequences of hydroxyl group location on the kinetics of *n*-hexane hydroisomerization over acidic zeolites pp 98–107

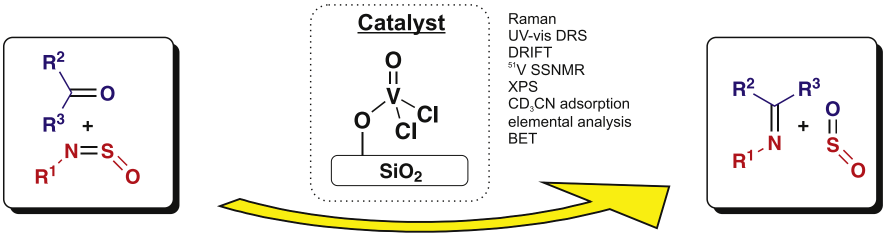
Hsu Chiang, Aditya Bhan*



The *n*-hexene molecule is partially confined in the 8-MR side pockets of MOR, which results in entropy of activation and selectivity for isomerization reactions in 8-MR pockets being similar to that in 12-MR channel zeolites; the lower activation energy in 8-MR channels results in catalytic rates per proton being five times higher than those in 12-MR channels of MOR.

Oxo/imido heterometathesis of *N*-sulfinylamines and carbonyl compounds catalyzed by silica-supported vanadium oxochloride pp 108–118

Pavel A. Zhizhko, Anton A. Zhizhin, Dmitry N. Zarubin*, Nikolai A. Ustynyuk, Dmitry A. Lemenovskii, Boris N. Shelimov,
Leonid M. Kustov, Olga P. Tkachenko, Gayane A. Kirakosyan



Grafting VOCl$_3$ onto silica surface gives well-defined vanadium surface complexes that are highly efficient heterogeneous catalysts for oxo/imido heterometathesis between *N*-sulfinylamines and carbonyl compounds.