Journal of Catalysis 284 (2011) iii–vi

Contents lists available at SciVerse ScienceDirect

Journal of Catalysis

journal homepage: www.elsevier.com/locate/jcat

Journal of Catalysis Vol. 284, Issue 2, 2011

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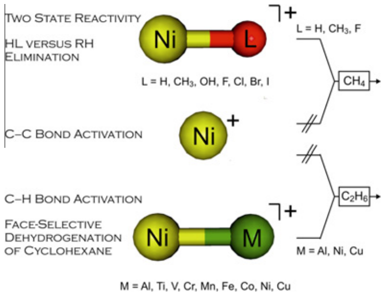
Molecular Approach to Heterogeneous Catalysis

Editorial for Special Issue of Journal of Catalysis on "Molecular Approach to Heterogeneous Catalysis" **pp 125**

Christophe Copéret

Probing elementary steps of nickel-mediated bond activation in gas-phase reactions: Ligand- and cluster-size effects **pp 126–137**

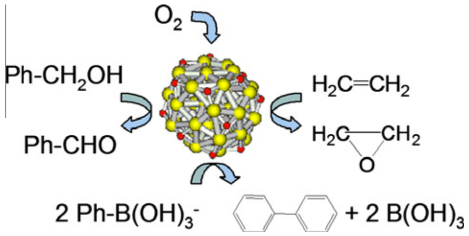
Maria Schlangen*, Helmut Schwarz*



With a little help from my friends: While "naked" Ni^+ is reluctant to bring about bond activation of small inert molecules, ligated species as well as nickel-containing dimeric clusters NiM^+ can activate methane and ethane, respectively. A summary of nickel chemistry in the gas phase is presented which is not only characterized by a remarkable reactivity that can be tuned by ligands over a broad scope, but also by a large diversity with respect to the reaction mechanisms observed for the individual gaseous nickel species.

Molecular approaches to catalysis. Naked gold nanoparticles as quasi-molecular catalysts for green processes **pp 138–147**

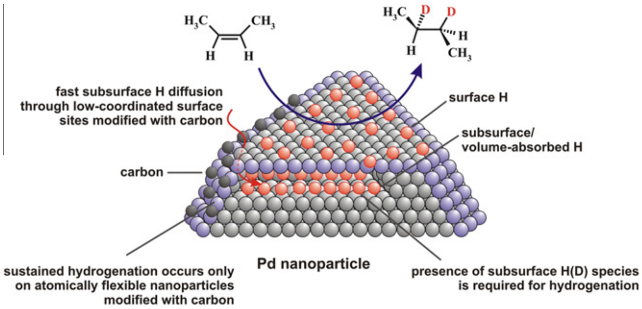
Mercedes Boronat, Avelino Corma*



Small gold nanoparticles can dissociate molecular O_2 and become reversibly oxidized. Different adsorbed oxygen species and low coordinated neutral and cationic gold sites are generated on the oxidized nanoparticles. The implication of these new sites in the mechanism of several reactions in which oxygen plays a crucial role is discussed.

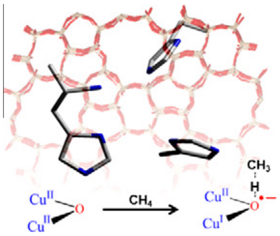
Olefin hydrogenation on Pd model supported catalysts: New mechanistic insights pp 148–156

Wiebke Ludwig, Aditya Savara, Karl-Heinz Dostert, Swetlana Schauermann*



Cu-ZSM-5: A biomimetic inorganic model for methane oxidation pp 157–164

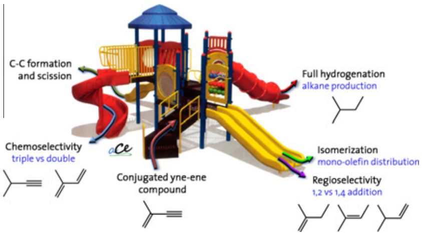
Pieter Vanelderen, Ryan G. Hadt, Pieter J. Smeets, Edward I. Solomon*, Robert A. Schoonheydt*, Bert F. Sels*



The present work highlights recent advances in elucidating the methane oxidation mechanism of the inorganic Cu-ZSM-5 biomimic and in identifying the reactive intermediates that are involved. Such understanding is important in view of upgrading abundantly available methane, but also to comprehend the working mechanism of genuine Cu-containing oxidation enzymes.

Selectivity patterns in heterogeneously catalyzed hydrogenation of conjugated ene-yne and diene compounds pp 165–175

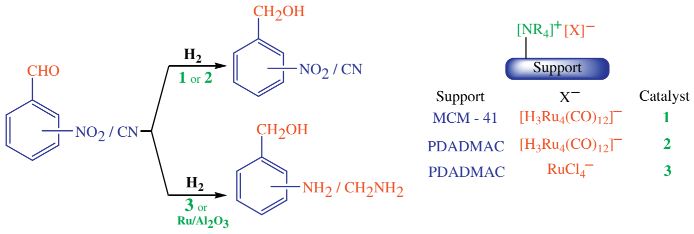
Blaise Bridier, Javier Pérez-Ramírez*



Selectivity patterns in the hydrogenation of conjugated ene-yne (valylene) and diene (isoprene) compounds are determined over Pd, Cu, and Ni-based catalysts.

Control of chemoselectivity in hydrogenations of substituted nitro- and cyano-aromatics by cluster-derived ruthenium nanocatalysts pp 176–183

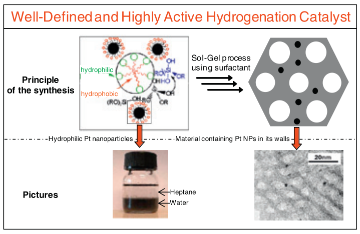
Arindam Indra, Niladri Maity, Prasenjit Maity, Sumit Bhaduri*, Goutam Kumar Lahiri*



Cluster-derived precatalysts **1** and **2** supported on MCM-41 and PDADMAC, [PDADMAC = water-soluble poly(diallyldimethylammonium chloride)], act as efficient and chemoselective hydrogenation catalysts for the reduction of nitrobenzaldehydes and cyano-benzaldehyde, whereas no such selectivity is observed either with PDADMAC-$RuCl_4$ (**3**) or with commercial (5%)Ru-Al_2O_3.

Selective and regular localization of accessible Pt nanoparticles inside the walls of an ordered silica: Application as a highly active and well-defined heterogeneous catalyst for propene and styrene hydrogenation reactions **pp 184–193**

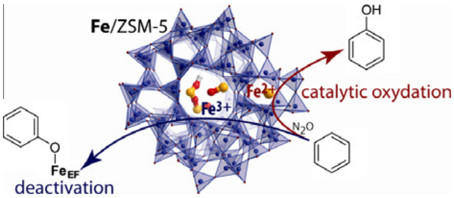
M. Boualleg, S. Norsic, D. Baudouin, R. Sayah, E.A. Quadrelli, J.-M. Basset, J.-P. Candy, P. Delichere, K. Pelzer, L. Veyre, C. Thieuleux*



Accessible 2 nm crystalline Pt(0) nanoparticles are localized by design in the walls of a highly ordered mesoporous oxide, by the use of novel hydrophilic preformed nanoparticles stabilized by chloroalkylsilane ligands. The embedded nanoparticles show no leaching nor sintering and are highly active in catalytic styrene and propene hydrogenations.

Stability and reactivity of active sites for direct benzene oxidation to phenol in Fe/ZSM-5: A comprehensive periodic DFT study **pp 194–206**

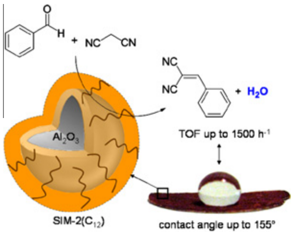
Guanna Li, Evgeny A. Pidko, Rutger A. van Santen, Zhaochi Feng, Can Li*, Emiel J.M. Hensen*



A periodic DFT study of the oxidation of benzene to phenol with N_2O by Fe/ZSM-5 zeolite has been carried out. The reaction is only catalytic over isolated Fe(II) cations. Mononuclear Fe(III) and binuclear Fe(II) and Fe(III) complexes also activate N_2O and benzene but lead to grafted phenolates that deactivate these iron sites.

Tuning the activity by controlling the wettability of MOF eggshell catalysts: A quantitative structure–activity study **pp 207–214**

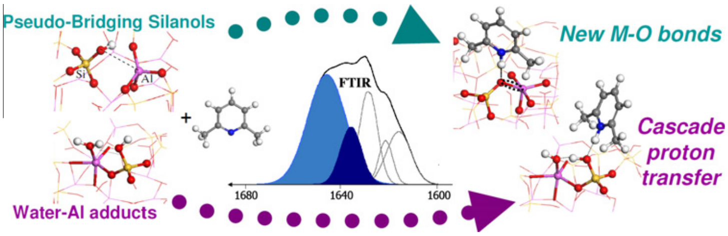
Sonia Aguado, Jerome Canivet, Yves Schuurman, David Farrusseng*



Well-controlled post-synthetic modification of an alumina-supported MOF, the SIM-1, allows the generation of genuine porous superhydrophobic material, the SIM-2. The later shows outstanding catalytic activity for the Knoevenagel reaction, TOF increasing with PSM yield.

Brønsted acidity of amorphous silica–alumina: The molecular rules of proton transfer **pp 215–229**

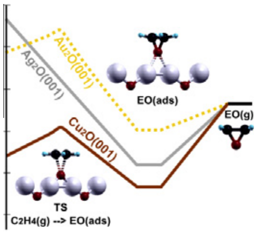
Fabien Leydier, Céline Chizallet, Alexandra Chaumonnot, Mathieu Digne, Emmanuel Soyer, Anne-Agathe Quoineaud, Dominique Costa, Pascal Raybaud*



Combined experiments and *first-principles* calculations unravel the nature and behavior of Brønsted acid sites on amorphous silica–alumina: the key roles of pseudo-bridging silanols and water molecules adsorbed on Al atoms are revealed.

Why silver is the unique catalyst for ethylene epoxidation pp 230–235

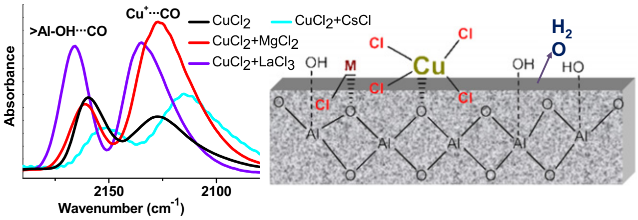
M.O. Ozbek, I. Onal, R.A. van Santen*



The difference in selectivity of ethylene epoxidation of Ag, Cu, and Au relates to the different reactivity of their oxidized surfaces. Au_2O is predicted to have the highest selectivity for ethylene oxide (EO) formation; however, catalytically it cannot be applied because O_2 will not regenerate the oxide. Cu_2O is found to activate ring opening EO with subsequent acetaldehyde formation. The latter barrier is higher than the desorption energy of EO on Ag_2O.

The role of chlorine and additives on the density and strength of Lewis and Brønsted acidic sites of γ-Al_2O_3 support used in oxychlorination catalysis: A FTIR study pp 236–246

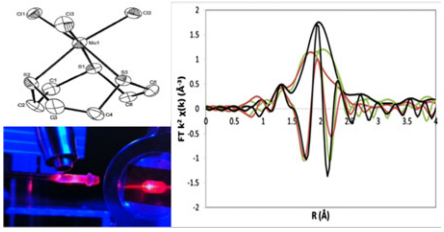
N.B. Muddada, U. Olsbye, T. Fuglerud, S. Vidotto, A. Marsella, S. Bordiga, D. Gianolio, G. Leofanti, C. Lamberti*



IR spectroscopy of adsorbed CO highlights that additives like $MgCl_2$, KCl, etc., used in industrial $CuCl_2/Al_2O_3$ catalysts for C_2H_4 oxychlorination, significantly modifies both the Lewis and the Brønsted acidity of the support, that in turns influences the electronic configuration of the active $CuCl_2$ phase.

Insights in the mechanism of selective olefin oligomerisation catalysis using stopped-flow freeze-quench techniques: A Mo K-edge QEXAFS study pp 247–258

Stuart A. Bartlett, Peter P. Wells, Maarten Nachtegaal, Andrew J. Dent, Giannantonio Cibin, Gillian Reid, John Evans, Moniek Tromp*



Time-resolved stopped-flow XAS in combination with a novel freeze-quench approach have established the stepwise alkylation of $[MoX_3(L)]$ complexes, analogous to the industrial $[CrX_3(L)]$ complexes for selective alkene oligomerisation reactions.