



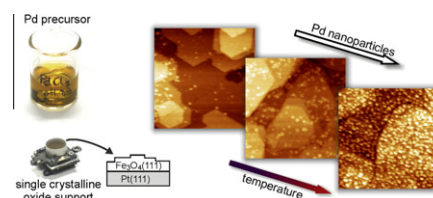
Contents

PRIORITY COMMUNICATION

Surface science approach to catalyst preparation – Pd deposition onto thin $\text{Fe}_3\text{O}_4(111)$ films from PdCl_2 precursor

pp 1–5

Hui-Feng Wang, Hiroko Ariga, Rhys Dowler, Martin Sterrer*, Hans-Joachim Freund



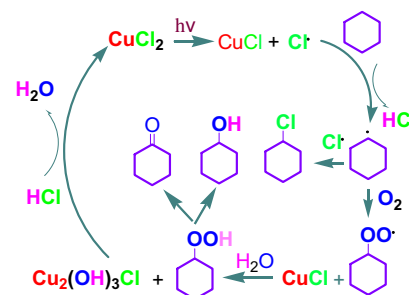
Utilizing thin, single-crystalline oxide films as substrate for model studies of supported metal catalyst preparation allows to track both morphological and chemical changes during the transformation of metal precursor complexes into nanoparticles.

REGULAR ARTICLES

Metal chlorides-catalyzed selective oxidation of cyclohexane by molecular oxygen under visible light irradiation

pp 6–12

Wenfeng Wu, Xiangling He, Zaihui Fu*, Yachun Liu*, Yanlong Wang, Xinglang Gong, Xiaolin Deng, Haitao Wu, Yanhong Zou, Ningya Yu, Dulin Yin

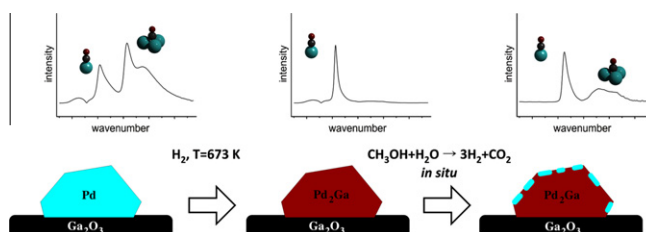


We found that acetone, like acetonitrile, was an efficient solvent for CuCl_2 -photocatalyzed cyclohexane oxidation with dioxygen, and the addition of concentrated HCl promoted this photocatalytic cycle, thus providing a high turnover number and good selectivity for the oxygenated products with using a low catalyst concentration and enhancing O_2 pressure.

In situ study of the formation and stability of supported Pd_2Ga methanol steam reforming catalysts

pp 13–21

Andreas Haghofer, Karin Föttinger*, Frank Girgsdies, Detre Teschner, Axel Knop-Gericke, Robert Schlögl, Günther Rupprechter

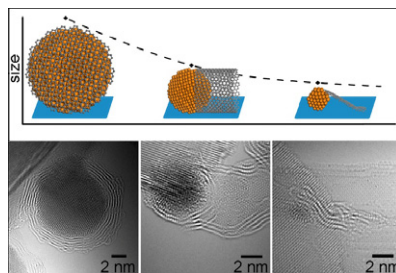


Supported Pd_2Ga is formed by reduction of $\text{Pd}/\text{Ga}_2\text{O}_3$. The bulk is structurally stable, its surface, however, is modified by O_2 already at RT leading to drastically reduced selectivity in MSR. Under MSR reaction conditions we propose the presence of a dynamic equilibrium between formation and decomposition of Pd_2Ga by the product H_2 and the byproduct CO , respectively, leading to a limited overall MSR selectivity.

High-resolution in situ and ex situ TEM studies on graphene formation and growth on Pt nanoparticles

pp 22–29

Zhenmeng Peng, Ferenc Somodi, Stig Helveg, Christian Kisielowski, Petra Specht, Alexis T. Bell*

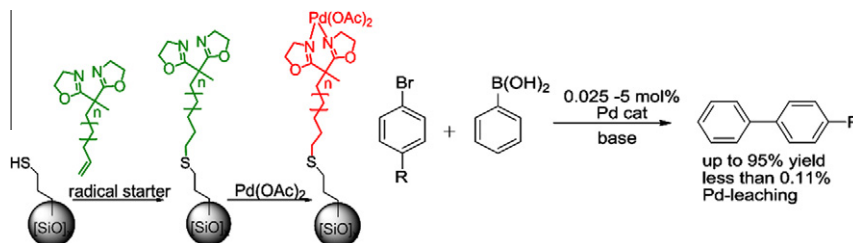


The formation of graphene layers on MgO-supported Pt nanoparticles was studied by both in situ and ex situ high-resolution transmission electron microscopy (HRTEM), which indicate that graphene sheets grow from steps in the surface of Pt nanoparticles and the subsequent morphology of the graphene sheets is a strong function of Pt particle size.

Synthesis, catalytic activity, and leaching studies of a heterogeneous Pd-catalyst including an immobilized bis(oxazoline) ligand

pp 30–40

H. Gruber-Woelfler, P.F. Radaschitz, P.W. Feenstra, W. Haas, J.G. Khinast*

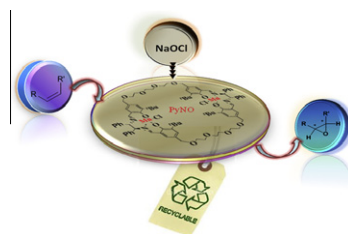


A catalytic system including a Pd(OAc)₂-bis(oxazoline) complex bonded to 3-mercaptopropyl-functionalized silica gel is presented. The catalyst was tested for Suzuki–Miyaura reactions. The heterogeneity of the catalytic system was studied indicating that there is virtually no Pd-leaching. Furthermore, the catalyst can be reused multiple times without significant loss of stability or structure.

Reusable chiral macrocyclic Mn(III) salen complexes for enantioselective epoxidation of nonfunctionalized alkenes

pp 41–50

Rukhsana I. Kureshy*, Tamal Roy, Noor-ul H. Khan, Sayed H.R. Abdi, Arghya Sadhukhan, Hari C. Bajaj

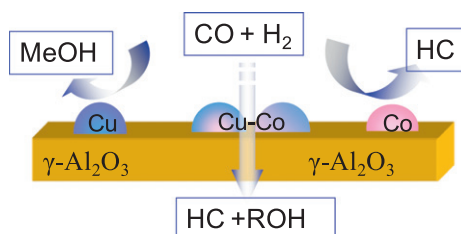


Chiral macrocyclic Mn(III) salen complexes catalyze the enantioselective epoxidation of nonfunctionalized alkenes with sodium hypochlorite in presence of several pyridine-*N*-oxide at 0 °C.

Structure and catalytic performance of alumina-supported copper–cobalt catalysts for carbon monoxide hydrogenation

pp 51–61

Jingjuan Wang, Petr A. Chernavskii, Andrei Y. Khodakov*, Ye Wang

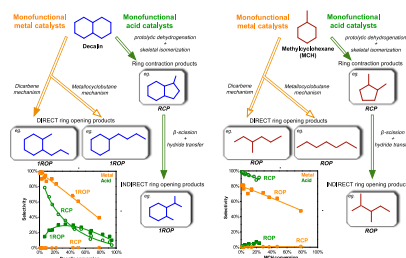


The alumina-supported copper–cobalt catalysts exhibit catalytic performance in carbon monoxide hydrogenation very different from that of monometallic counterparts. The catalytic and characterization results are interpreted in terms of formation of bimetallic particles in the activated catalysts.

Ring opening of decalin and methylcyclohexane over alumina-based monofunctional WO_3/Al_2O_3 and Ir/Al_2O_3 catalysts

pp 62–77

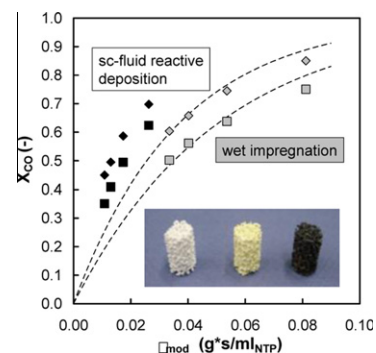
Rodrigo Moraes, Karine Thomas, Sébastien Thomas, Sander Van Donk, Giacomo Grasso, Jean-Pierre Gilson, Marwan Houalla*



Novel $PtCuO/CeO_2/\alpha-Al_2O_3$ sponge catalysts for the preferential oxidation of CO (PROX) prepared by means of supercritical fluid reactive deposition (SFRD)

pp 78–87

Sebastian Lang, Michael Türk, Bettina Kraushaar-Czarnetzki*

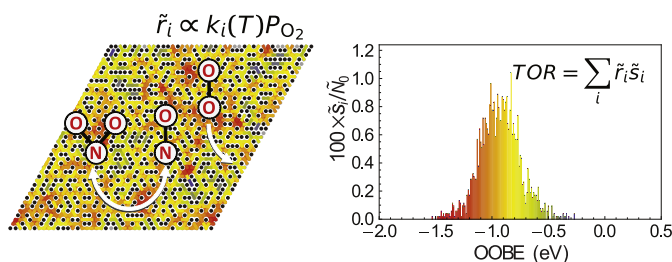


Novel PROX-catalysts on ceramic sponges prepared via supercritical fluid reactive deposition outperform catalysts prepared via conventional routes.

Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt (1 1 1)

pp 88–94

C. Wu, D.J. Schmidt, C. Wolverton, W.F. Schneider*

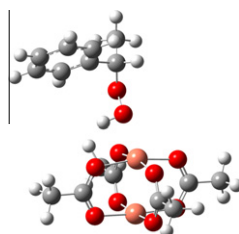


A DFT-based cluster expansion (CE) combined with Monte Carlo simulations is used to accurately describe the heterogeneous distribution of adsorbates and O_2 dissociation sites at a Pt (1 1 1) surface under realistic NO oxidation conditions. O_2 dissociation rates are sensitive to the local arrangement of adsorbates, and averaging over these arrangements provides reaction rates and rate derivatives in good agreement with experiment.

DFT investigation of hydroperoxide decomposition over copper and cobalt sites within metal-organic frameworks

pp 95–102

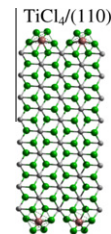
Patrick Ryan, Ivan Konstantinov, Randall Q. Snurr*, Linda J. Broadbelt*



Density functional theory calculations were performed for hydroperoxide decomposition over metal clusters found in metal-organic frameworks. The calculations suggest that in some cases, constraints of the framework prevent metals in the MOF interior from catalyzing this reaction.

A periodic hybrid DFT approach (including dispersion) to MgCl_2 -supported Ziegler–Natta catalysts – 1: TiCl_4 adsorption on MgCl_2 crystal surfaces pp 103–110

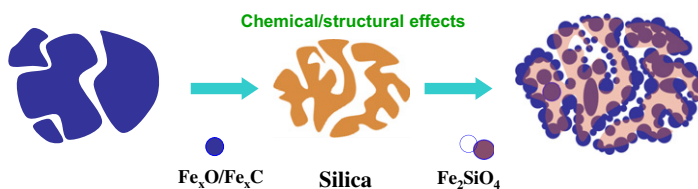
Maddalena D'Amore*, Raffaele Credendino, Peter H.M. Budzelaar, Mauro Causá, Vincenzo Busico



The adsorption of TiCl_4 on the surfaces of MgCl_2 crystals has been investigated by means of state-of-the-art periodic hybrid DFT methods (B3LYP(-D), PBE0(-D) and M06 approximations). The inclusion of dispersion forces turned out to be crucial for a correct analysis of the problem: the phenomenon is essentially dispersion-driven. Under conditions representative of precatalyst preparation, TiCl_4 can only adsorb on $\text{MgCl}_2(1\ 1\ 0)$; with respect to the indication of a preferential binding to $\text{MgCl}_2(1\ 0\ 4)$, the present DFT investigation is negative.

Chemical and structural effects of silica in iron-based Fischer–Tropsch synthesis catalysts pp 111–123

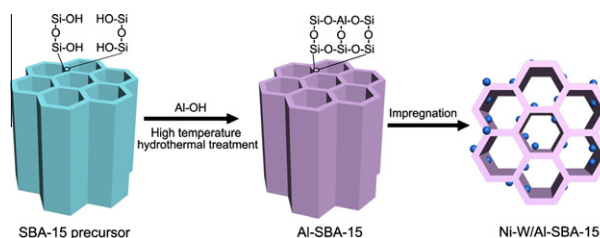
Haiyun Suo, Shengguang Wang, Chenghua Zhang*, Jian Xu, Baoshan Wu, Yong Yang, Hongwei Xiang, Yong-Wang Li



Silica affects iron Fischer–Tropsch catalysts in several ways. As a chemical promoter, it inhibits reduction and carburization of the iron, while in structural sense, it improves the iron dispersion and stabilizes the active phase. Finally, it suppresses the formation of methane.

Synthesis and hydrodesulfurization properties of NiW catalyst supported on high-aluminum-content, highly ordered, and hydrothermally stable Al-SBA-15 pp 124–136

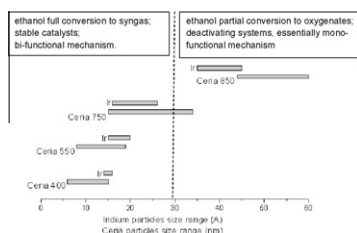
Yang Li, Dahai Pan, Chengzhong Yu*, Yu Fan, Xiaojun Bao*



Al-SBA-15 was prepared by adjusting the pH value during high-temperature hydrothermal treatment. Appropriate metal–support interaction combined with suitable acidity endowed the NiW/Al-SBA-15 catalyst with excellent hydrodesulfurization activity.

Oxidative steam reforming of ethanol over Ir/CeO₂ catalysts: A structure sensitivity analysis pp 137–152

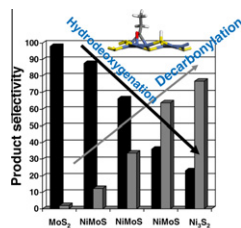
Weijie Cai, Fagen Wang, Cécile Daniel, Andre C. van Veen, Yves Schuurman, Claude Descorme, Hélène Provendier, Wenjie Shen*, Claude Mirodatos*



Deoxygenation mechanisms on Ni-promoted MoS₂ bulk catalysts: A combined experimental and theoretical study

pp 153–164

M. Ruinat de Brimont, C. Dupont, A. Daudin*, C. Geantet, P. Raybaud



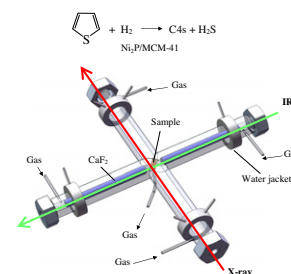
The deoxygenation pathways of ester depend on the nature of the transition metal sulfide bulk catalyst: MoS₂-based catalysts favor hydrodeoxygenation, whereas the decarbonylation selectivity increases as a function of the Ni monosulfide content; a rational interpretation is furnished by DFT calculations.

Combined in situ QXAFS and FTIR analysis of a Ni phosphide catalyst under hydrodesulfurization conditions

pp 165–171

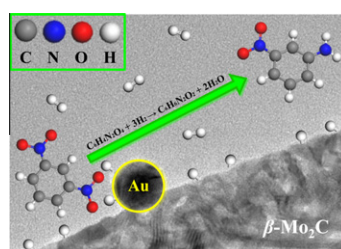
Kyoko K. Bando*, Takahiro Wada, Takeshi Miyamoto, Kotaro Miyazaki, Satoru Takakusagi, Yuichiro Koike, Yasuhiro Inada, Masaharu Nomura, Aritomo Yamaguchi, Travis Gott, S. Ted Oyama, Kiyotaka Asakura*

Simultaneous X-ray absorption spectroscopy and transmission Fourier transform infrared spectroscopy were applied to study the mechanism of thiophene hydrodesulfurization over Ni₂P/MCM-41. The measurements were carried out at transient conditions using quick X-ray absorption with a limiting spectral acquisition time of 10 s. The studies showed that a phosphosulfide was the active species and that a tetrahydrothiophene intermediate was involved in the reaction.

**Enhanced selective nitroarene hydrogenation over Au supported on β-Mo₂C and β-Mo₂C/Al₂O₃**

pp 172–183

Noémie Perret, Xiaodong Wang, Laurent Delannoy, Claude Potvin, Catherine Louis, Mark A. Keane*

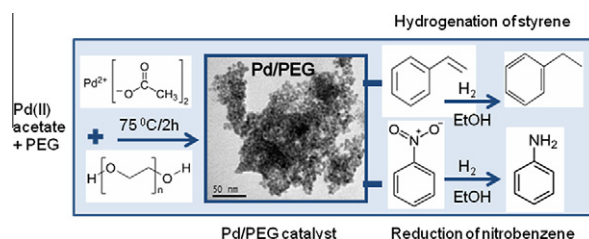


Au/β-Mo₂C promotes hydrogenation of dinitrobenzene with exclusive production of nitroaniline.

Palladium nanoparticles stabilized by polyethylene glycol: Efficient, recyclable catalyst for hydrogenation of styrene and nitrobenzene

pp 184–192

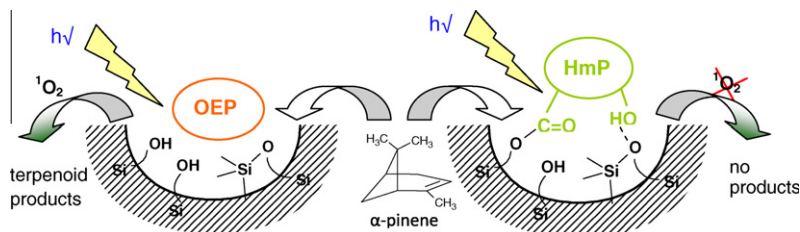
F.A. Harraz*, S.E. El-Hout, H.M. Killa, I.A. Ibrahim



Sol-gel immobilization of octaethylporphine and hematoporphyrin for biomimetic photooxidation of α -pinene

pp 193–205

Mariusz Trytek*, Marek Majdan, Agnieszka Lipke, Jan Fiedurek

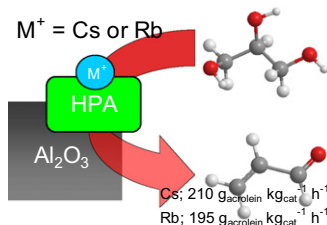


Octaethylporphine (OEP) and hematoporphyrin (HmP) immobilized in pore silica gel show good luminescent properties, but biocatalytic activity in the photoconversion of α -pinene is only found for OEP/SiO₂. It is suggested that the blocking of silanol/siloxane groups by electrophilic substituents of HmP prevents transfer of energy for the formation of reactive oxygen species.

Rubidium- and caesium-doped silicotungstic acid catalysts supported on alumina for the catalytic dehydration of glycerol to acrolein

pp 206–213

Muhammad H. Haider, Nicholas F. Dummer, Dazhi Zhang, Peter Miedziak, Thomas E. Davies, Stuart H. Taylor, David J. Willock, David W. Knight, David Chadwick, Graham J. Hutchings*

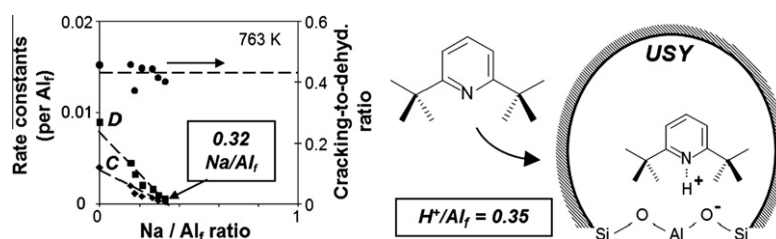


Dehydration of glycerol to acrolein was carried out using rubidium- and caesium-doped silicotungstic acid catalysts supported on alumina. Cs-doped silicotungstic acid supported on theta-delta alumina gave a maximum selectivity of ca. 90% at 100% glycerol conversion and with a more concentrated glycerol feed (20 wt.%) achieved a space time yield of 210 g_(acrolein) kg_(cat)⁻¹ h⁻¹. The catalysts were tested for up to 200 h on-stream and found to be stable for 90 h (10 wt.% glycerol).

Solvation and acid strength effects on catalysis by faujasite zeolites

pp 214–223

Rajamani Gounder, Andrew J. Jones, Robert T. Carr, Enrique Iglesia*

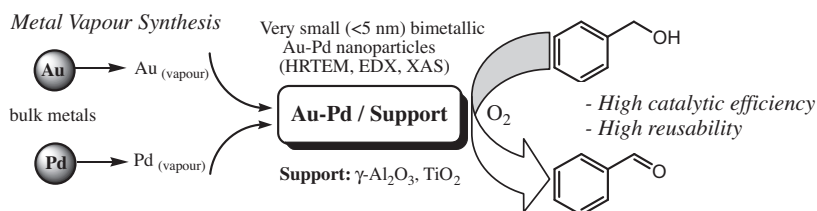


Demystifying faujasite: Isobutane cracking (C) and dehydrogenation (D) rate constants (per framework Al; Al_I), but not their ratio, decreased monotonically with Na⁺ content in ultrastable Y (USY) zeolite. Similar Na⁺ and 2,6-di-*tert*-butylpyridine titrant uptakes completely suppressed catalytic rates, indicating that there are fewer H⁺ sites than Al_I atoms and that Na⁺ stoichiometrically replaces H⁺ sites that are uniform in reactivity and acid strength.

Bimetallic Gold–Palladium vapour derived catalysts: The role of structural features on their catalytic activity

pp 224–236

Claudio Evangelisti*, Eleonora Schiavi, Laura Antonella Aronica, Anna Maria Caporusso, Giovanni Vitulli, Luca Bertineti, Gianmario Martra, Antonella Balerna, Settimio Mobilio

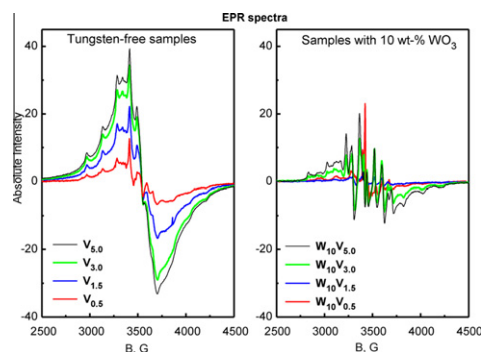


New supported Au–Pd bimetallic catalysts were easily synthesized starting from Au–Pd/acetone solutions generated according to the metal vapour synthesis technique. Transmission electron microscopy (TEM) and X-ray absorption spectroscopy (XAS) analyses on supported systems showed very small (<5 nm) bimetallic Au–Pd nanoparticles and very narrow size distributions. The catalytic efficiency of supported Au–Pd systems was tested in the selective oxidation of benzyl alcohol with molecular oxygen evidencing the role of the structural features on their catalytic activity and selectivity.

A new view on the relations between tungsten and vanadium in $V_2O_5WO_3/TiO_2$ catalysts for the selective reduction of NO with NH_3

pp 237–247

Patrick G.W.A. Kompio, Angelika Brückner, Frank Hipler, Gerhard Auer, Elke Löffler, Wolfgang Grünert*

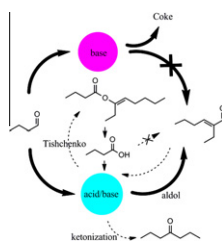


In spontaneous arrangement of surface V and W oxide species on anatase, a well-mixed surface oxide phase is formed, with surface W oxide species preventing the formation of extended two-dimensional vanadium oxide islands.

Vapor phase butanal self-condensation over unsupported and supported alkaline earth metal oxides

pp 248–259

Wenqin Shen, Geoffrey A. Tompsett, Rong Xing, W. Curtis Conner Jr., George W. Huber*

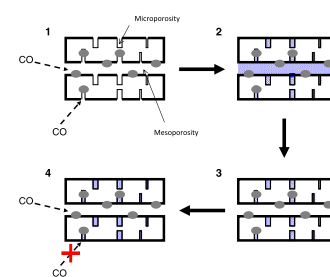


Vapor phase butanal condensation was studied over well-characterized solid base catalyst MgO, and silica supported MgO, SrO and MgOSrO and MgO/HY in a fixed-bed flow reactor. The silica supported MgO, SrO and MgOSrO and MgO/HY had almost a five times higher activity and a higher stability compared to the unsupported MgO indicating that both acid and base sites are needed to achieve good catalytic performance.

Understanding the spatial distribution of coke deposition within bimodal micro-/mesoporous catalysts using a novel sorption method in combination with pulsed-gradient spin-echo NMR

pp 260–265

Li Min Chua, Iain Hitchcock, Robin S. Fletcher, Elizabeth M. Holt, John Lowe, Sean P. Rigby*

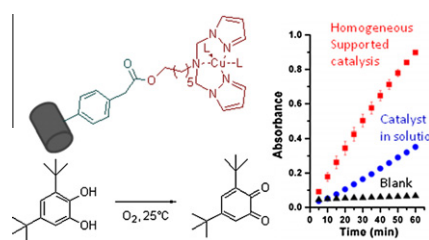


Determination of the spatial location of metal surface area within bidisperse, MFI zeolite-based catalysts.

Continuous flow catalysis with a biomimetic copper(II) complex covalently immobilized on graphite felt

pp 266–272

Ronan Marion, Gopinathan Muthusamy, Florence Geneste*

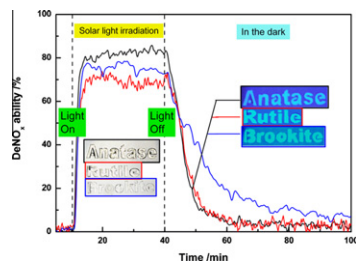


The catecholase activity of a copper(II) complex coordinated by a *N*-tripodal pyrazole-based ligand is investigated in continuous flow catalysis. The complex is covalently immobilized on a graphite felt in two steps. First, the surface is derivatized by electrochemical reduction of 4-carboxymethyl-benzenediazonium salts. Second the complex is attached onto the support via an esterification reaction. A better catalytic activity is obtained in homogeneous supported catalysis with 50 times less catalyst than when it is in solution.

Effect of phase structures of $\text{TiO}_2\text{-xN}_y$ on the photocatalytic activity of $\text{CaAl}_2\text{O}_4\text{:}(\text{Eu}, \text{Nd})\text{-coupled TiO}_2\text{-xN}_y$

pp 273–278

Huihui Li*, Shu Yin, Yuhua Wang, Tsugio Sato

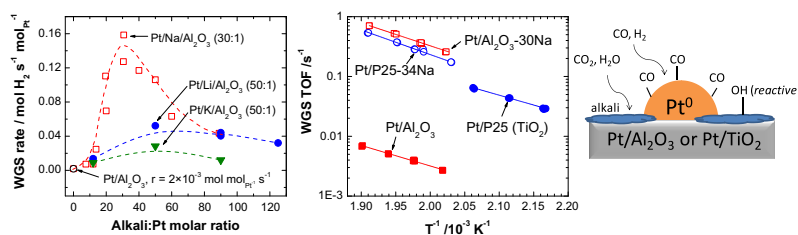


Nitrogen doping of TiO_2 and coupling it with a fluorescent material induces persistent photocatalytic activity even after switching off the light.

Metallic Pt as active sites for the water–gas shift reaction on alkali-promoted supported catalysts

pp 279–286

Jorge H. Pazmiño, Mayank Shekhar, W. Damion Williams, M. Cem Akatay, Jeffrey T. Miller, W. Nicholas Delgass, Fabio H. Ribeiro*

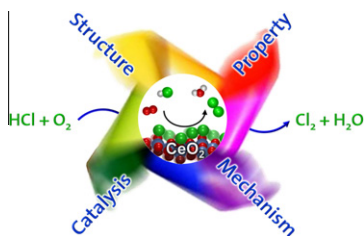


The enhancement of the WGS rate by alkali components (Li, Na, and K) was confirmed on $\text{Pt}/\text{Al}_2\text{O}_3$. Addition of sodium resulted in the highest promotion. Upon addition of Na, the rate and kinetics of Pt/TiO_2 were similar to $\text{Pt}/\text{Al}_2\text{O}_3$. Promoted samples showed fully reduced Pt under reaction conditions. The promotion by alkali is therefore caused by the modification of the support and not the nature of Pt.

Performance, structure, and mechanism of CeO_2 in HCl oxidation to Cl_2

pp 287–297

Amol P. Amrute, Cecilia Mondelli, Maximilian Moser, Gerard Novell-Leruth, Núria López, Dirk Rosenthal, Ramzi Farra, Manfred E. Schuster, Detre Teschner, Timm Schmidt, Javier Pérez-Ramírez*



CeO_2 is a promising catalytic system for industrial use in HCl oxidation. Experimental and theoretical studies reveal performance descriptors and provide molecular-level understanding of the reaction over this intriguing oxide.

CORRIGENDA**Corrigendum to “Improvement of the photocatalytic hydrogen evolution activity of $\text{Sm}_2\text{Ti}_2\text{S}_2\text{O}_5$ under visible light by metal ion additives” [J. Catal. 280 (2011) 1–7]**

p 298

Fuxiang Zhang, Kazuhiko Maeda, Tsuyoshi Takata, Kazunari Domen*

Corrigendum to “Methane oxidation on Pd–Ceria: A DFT study of the mechanism over Pd_xCe_{1-x}O₂, Pd, and PdO”
[J. Catal. 2781 (2011) 16–25]

p 299

Adam D. Mayernick, Michael J. Janik*
