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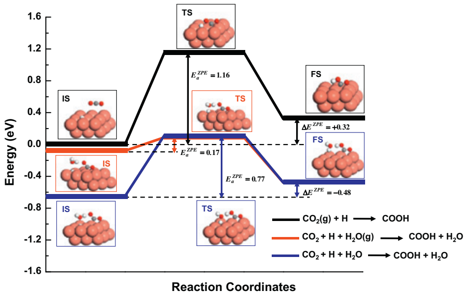
## Journal of Catalysis Vol. 281, Issue 2, 2011

# Contents

## REGULAR ARTICLES

### Insight into methanol synthesis from $CO_2$ hydrogenation on Cu(1 1 1): Complex reaction network and the effects of $H_2O$ pp 199–211

Ya-Fan Zhao, Yong Yang, Charles Mims, Charles H.F. Peden, Jun Li, Donghai Mei*



In the presence of $H_2O$, the *trans*-COOH formation is dramatically facilitated by a unique hydrogen transfer mechanism. The weakly bonded $CO_2$ is hydrogenated by one of the H atoms in $H_2O$ while the atomic surface H begins to interact strongly with the $H_2O$ molecule.

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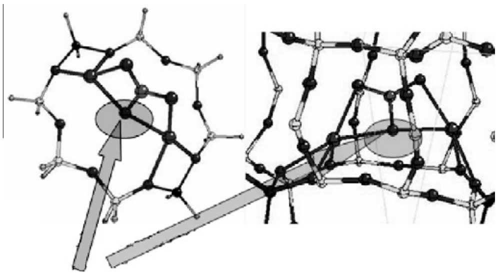
### Oxide clusters as source of the third oxygen atom for the formation of carbonates in alkaline earth dehydrated zeolites pp 212–221

Alexander V. Larin*, Andrey A. Rybakov, Georgii M. Zhidomirov, Amber Mace, Aatto Laaksonen, Daniel P. Vercauteren



Cluster and periodic type *QM* optimizations of the 3D structures and evaluations of the IR spectra confirm that the oxygen atoms of metal oxide species participate in the formation of carbonates in zeolites.

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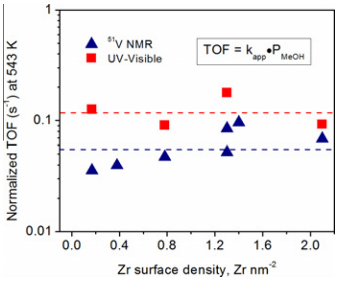
### Investigation of the structure and activity of $VO_x/ZrO_2/SiO_2$ catalysts for methanol oxidation to formaldehyde pp 222–230

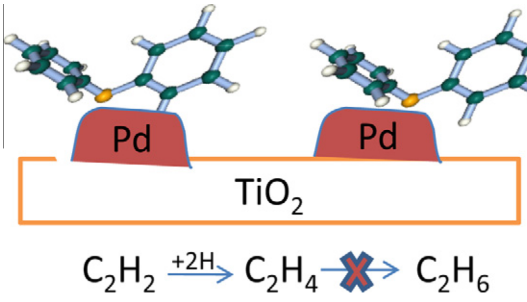
William C. Vining, Jennifer Strunk, Alexis T. Bell*



Methanol oxidation on bilayered $VO_x/ZrO_2/SiO_2$ catalysts was investigated. The catalysts were shown to exist in both O=V(O–Si)$_3$ and O=V(O–Zr)$_3$ environments with an increasing fraction of the latter with increasing Zr surface density. A constant TOF was obtained when the rate was normalized to the number of O=V(O–Zr)$_3$ sites, which are the active sites for methanol oxidation on these bilayered catalysts.

### Selectivity enhancement in acetylene hydrogenation over diphenyl sulphide-modified Pd/$TiO_2$ catalysts pp 231–240

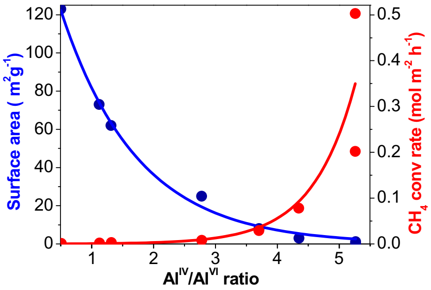
Fiona-Mairead McKenna, James A. Anderson*



Diphenylsulfide and its sulfur residue was found to modify Pd/$TiO_2$ catalysts leading to significantly enhanced selectivity in acetylene hydrogenation in the presence of ethylene.

### SrO·$Al_2O_3$ mixed oxides: A promising class of catalysts for oxidative coupling of methane pp 241–253

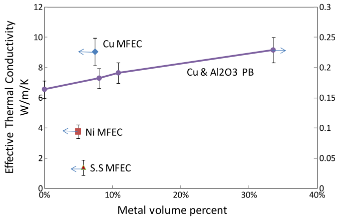
Tinku Baidya, Niels van Vegten, René Verel, Yijiao Jiang, Maxim Yulikov, Thomas Kohn, Gunnar Jeschke, Alfons Baiker*



Methane conversion rate increases exponentially with increasing ratio of tetrahedral $Al^{IV}$ to octahedral $Al^{VI}$ sites while surface area decreases, indicating higher population density or higher activity of sites at higher $Al^{IV}/Al^{VI}$.

### Novel catalyst structures with enhanced heat transfer characteristics pp 254–262

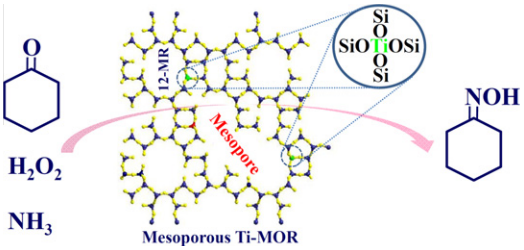
Min Sheng, Hongyun Yang, Donald R. Cahela, Bruce J. Tatarchuk*



Microfibrous entrapped catalyst (MFEC) was addressed to improve the intra-bed heat transfer for highly exothermic and endothermic reactions, as proved in Fischer–Tropsch synthesis. The thermal conductivity of Cu MFEC is 56-fold of that of traditional alumina-packed bed, while the inside wall heat transfer coefficient is 10 times higher.

### Postsynthesis of mesoporous MOR-type titanosilicate and its unique catalytic properties in liquid-phase oxidations pp 263–272

Hao Xu, Yingtian Zhang, Haihong Wu*, Yueming Liu, Xiaohong Li, Jingang Jiang, Mingyuan He, Peng Wu*



Mesoporous titanosilicate with the MOR topology, postsynthesized by sequential dealumination, desilication, and $TiCl_4$ vapor treatment, are highly active for the liquid-phase ammoximation of cyclohexanone and hydroxylation of toluene with hydrogen peroxide as oxidant.

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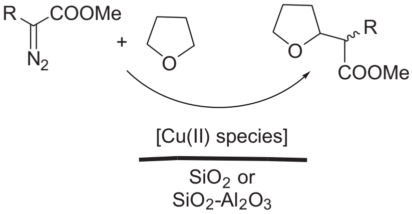
**Heterogeneous catalysts for carbene insertion reactions** **pp 273–278**

José M. Fraile*, José A. Mayoral, Nicoletta Ravasio, Marta Roldán, Laura Sordelli, Federica Zaccheria



Cu(II)/$SiO_2$–$Al_2O_3$ is an efficient and recoverable catalyst for carbene insertions into THF.

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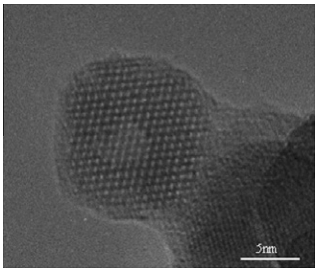
**The effect of heat treatment on phase formation of copper manganese oxide: Influence on catalytic activity for ambient temperature carbon monoxide oxidation** **pp 279–289**

Simon A. Kondrat, Thomas E. Davies, Zhongling Zu, Paul Boldrin, Jonathan K. Bartley, Albert F. Carley, Stuart H. Taylor, Matthew J. Rosseinsky, Graham J. Hutchings*



The auto-reduction of copper and manganese acetates has been manipulated, to tailor specific Cu/Mn/O phases for the purpose of investigating their relation to activity for CO oxidation. A range of phases were produced from Hopcalite to discrete metallic copper particles supported by manganese oxide. The Hopcalite spinel phase was found to be required for the activity, while copper and manganese oxides were found to be inactive.

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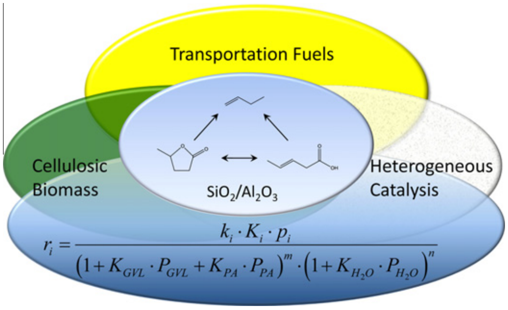
**Interconversion between γ-valerolactone and pentenoic acid combined with decarboxylation to form butene over silica/alumina** **pp 290–299**

Jesse Q. Bond, Dong Wang, David Martin Alonso, James A. Dumesic*



The conversion of γ-valerolactone over $SiO_2/Al_2O_3$ for the production of butenes or pentenoic acid represents an important application of heterogeneous catalysis in bio-refining practice. In this study, we present a reaction kinetics study of key transformations and provide a simple kinetic model that captures the reactivity trends

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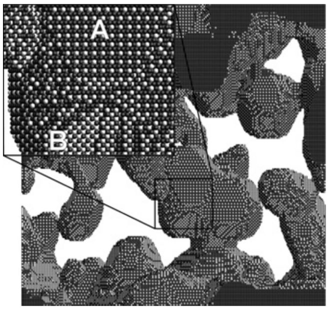
**A quantitative investigation of the structure of Raney-Ni catalyst material using both computer simulation and experimental measurements** **pp 300–308**

N.C. Barnard, S.G.R. Brown*, F. Devred, J.W. Bakker, B.E. Nieuwenhuys, N.J. Adkins



Monte Carlo modelling is used to simulate the 3D nano-porous structure of leached Raney-nickel catalyst material. Calculated surface areas from the model compare favourably to measured surface areas from BET analysis and also predict surface segregation of residual Al matching X-ray photoelectron spectroscopy results. In the figure, the magnified view at the top left shows a region (A), which is an exposed (1 1 1) plane and a region below (B), which is an exposed (1 0 0) plane. Dark atoms are Ni and light atoms are Al.

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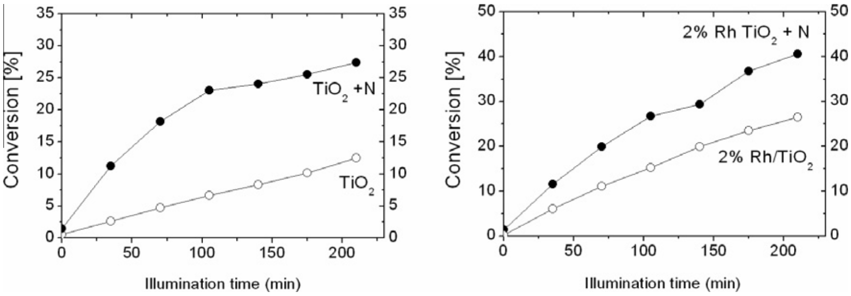
### Photocatalytic decomposition of ethanol on $TiO_2$ modified by N and promoted by metals pp 309–317

Gyula Halasi, Imre Ugrai, Frigyes Solymosi*



Modification of $TiO_2$ with N, through the decrease of the bandgap, enhances the extent of photodecomposition of ethanol on $TiO_2$ and Rh/$TiO_2$ even in the visible light.

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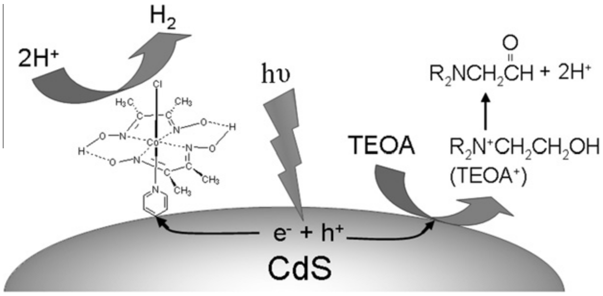
### Photocatalytic $H_2$ production on hybrid catalyst system composed of inorganic semiconductor and cobaloximes catalysts pp 318–324

Fuyu Wen, Jinhui Yang, Xu Zong, Baojun Ma, Donge Wang, Can Li*



An artificial photocatalytic system mimicking photosystem I (PSI) has been assembled using semiconductor (CdS) as the photosensitizer, cobaloximes ($Co^{III}$ complexes) as the $H_2$ evolution catalysts, and triethanolamine (TEOA) as the sacrificial electron donor. This artificial photocatalytic system shows high hydrogen evolution activity (TON up to 171 based on $Co^{III}(dmgH)_2pyCl$) under visible light irradiation.

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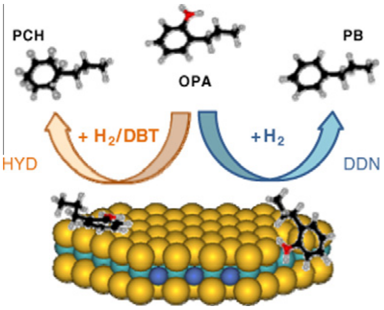
### Selective poisoning of the direct denitrogenation route in o-propylaniline HDN by DBT on Mo and NiMo/γ-$Al_2O_3$ sulfide catalysts pp 325–338

Ana Hrabar, Jennifer Hein, Oliver Y. Gutiérrez, Johannes A. Lercher*



The HDN of o-propylaniline on $MoS_2$/γ-$Al_2O_3$ and NiMoS/γ-$Al_2O_3$ catalysts proceeds via two parallel routes on two separate sites. Direct denitrogenation (DDN) is catalyzed only by accessible Mo cations, while the sites at the basal plane near the edge of the sulfide slabs (brim sites) are active for hydrogenation (HYD).

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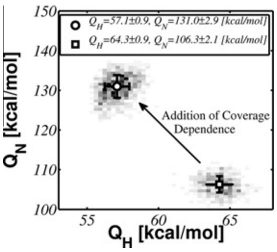
### Effect of multiscale model uncertainty on identification of optimal catalyst properties pp 339–344

Z. Ulissi, V. Prasad, D.G. Vlachos*



Uncertainty in kinetic parameters results in a distribution of optimal binding energies with an average and a standard deviation within which materials should be tested for best performance. Adsorbate–adsorbate interactions can strongly affect the optimal material properties of ammonia decomposition and thus the materials selection.

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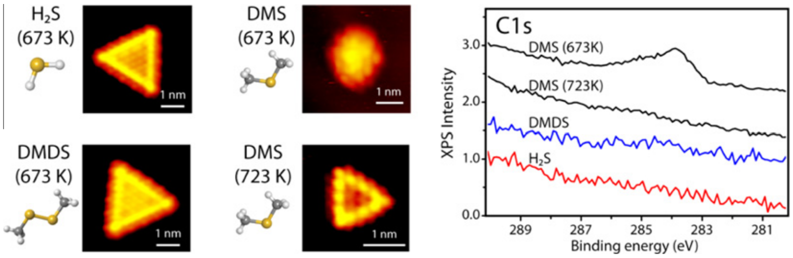
**An atomic-scale investigation of carbon in $MoS_2$ hydrotreating catalysts sulfided by organosulfur compounds** **pp 345–351**

Anders Tuxen, Henrik Gøbel, Berit Hinnemann, Zheshen Li, Kim G. Knudsen, Henrik Topsøe, Jeppe V. Lauritsen*, Flemming Besenbacher



From Scanning Tunneling Microscopy (STM), X-ray Photoelectron Spectroscopy (XPS) experiments, and density functional theory (DFT) calculations, we reveal that incorporation of carbon in $MoS_2$-based hydrotreating catalysts as carbide-type phase is not favorable when synthesized with or exposed to dimethyl disulfide (DMDS) or dimethyl sulfide (DMS).

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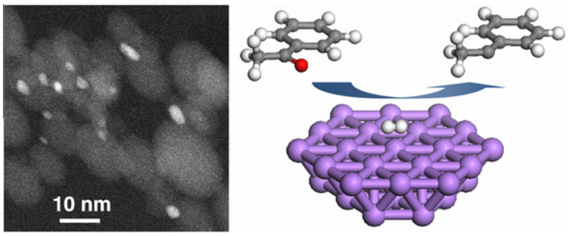
**Tuning the support acidity of flame-made $Pd/SiO_2–Al_2O_3$ catalysts for chemoselective hydrogenation** **pp 352–360**

Jun Huang, Yijiao Jiang, Niels van Vegten, Michael Hunger, Alfons Baiker*



Depending on the Si/Al ratio, flame-made Pd/silica–alumina showed tunable acidity, as evidenced by MAS NMR. Catalysts with moderate acidity show high chemoselectivity for hydrogenation of the carbonyl group of acetophenone, while high support acidity favors hydrogenation of the aromatic ring.

## ERRATA

**Erratum to "New efficient and long life catalyst for gas-phase glycerol dehydration to acrolein" [J. Catal. 280 (2011) 68–76]** **p 361**

P. Lauriol-Garbey, J.M.M. Millet*, S. Loridant, V. Bellière-Baca, P. Rey

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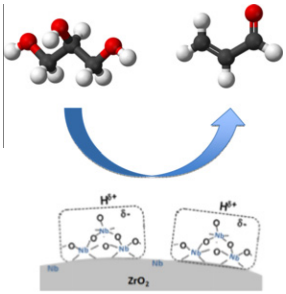
**New efficient and long-life catalyst for gas-phase glycerol dehydration to acrolein** **pp 362–370**

P. Lauriol-Garbey, J.M.M. Millet*, S. Loridant, V. Bellière-Baca, P. Rey



Zirconium and niobium mixed oxides have been shown to be selective catalysts for dehydration of glycerol to acrolein, at 300 °C in gas phase. The catalysts exhibit a selectivity to acrolein of approximately 72%, at nearly total glycerol conversion The New catalysts distinguish themselves by their unique stability on stream that make them promising for industrial application.

## CORRIGENDUM