



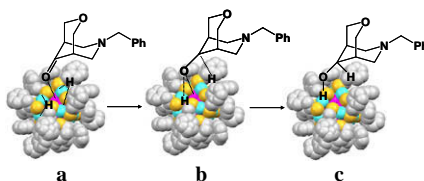
## Contents

## PRIORITY COMMUNICATION

Exploring stereoselectivity of Au<sub>25</sub> nanoparticle catalyst for hydrogenation of cyclic ketone

pp 155–160

Yan Zhu, Zhikun Wu, Chakicherla Gayathri, Huifeng Qian, Roberto R. Gil, Rongchao Jin\*



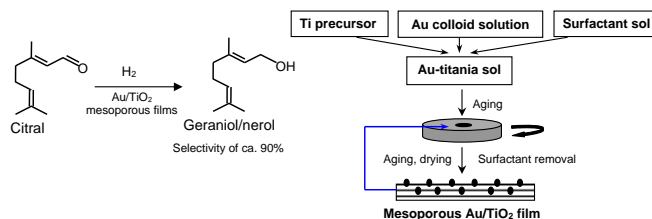
Atomically monodisperse Au<sub>25</sub>(SR)<sub>18</sub> (R=CH<sub>2</sub>CH<sub>2</sub>Ph) nanoparticles are explored as a new type of stereoselective catalyst for hydrogenation of cyclic ketone to a specific isomer of the cyclic alcohol product. A complete (100%) stereoselectivity is obtained and the catalytic performance is further correlated with the crystal structure of the Au<sub>25</sub>(SR)<sub>18</sub> nanoparticle.

## REGULAR ARTICLES

## Control of the thickness of mesoporous titania films for application in multiphase catalytic microreactors

pp 161–169

Lidia N. Protasova, Evgeny V. Rebrov, Tatiana S. Glazneva, Angel Berenguer-Murcia, Zinifer R. Ismagilov, Jaap C. Schouten\*

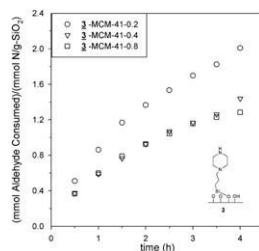


Control of the thickness of mesoporous Au/TiO<sub>2</sub> films was achieved by multiple spin-coating. A 300 nm thick Au-containing film showed high initial TOF of 1.4 s<sup>-1</sup> and a selectivity towards unsaturated alcohols as high as 90% in the hydrogenation of citral.

## Nitroaldol reactions catalyzed by amine-MCM-41 hybrids

pp 170–177

Qingqing Wang, Daniel F. Shantz\*

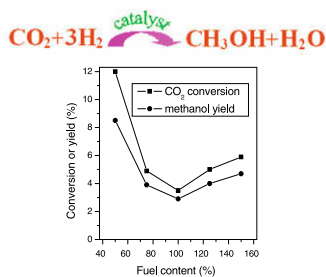


Amine-functionalized amine-MCM-41 materials were investigated as catalysts for the nitroaldol reaction. The secondary amines investigated were generally more active than primary amines.

**Glycine–nitrate combustion synthesis of CuO–ZnO–ZrO<sub>2</sub> catalysts for methanol synthesis from CO<sub>2</sub> hydrogenation**

pp 178–185

Xiaoming Guo, Dongsen Mao\*, Guanzhong Lu\*, Song Wang, Guisheng Wu

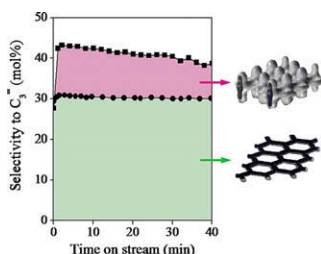


The fuel content used for the preparation of CuO–ZnO–ZrO<sub>2</sub> catalysts by combustion method had significant effect on CO<sub>2</sub> conversion and methanol yield for the synthesis of methanol from CO<sub>2</sub> hydrogenation.

**Methanol-to-olefin conversion over H-MCM-22 and H-ITQ-2 zeolites**

pp 186–194

Hyung-Ki Min, Min Bum Park, Suk Bong Hong\*

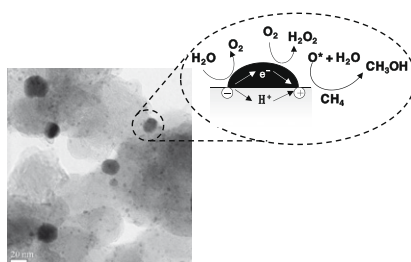


The contribution of 2-D sinusoidal 10-ring channels in H-MCM-22 to the overall MTO performance of this medium-pore zeolite was found to be considerably greater than that of its cylindrical supercages.

**Direct oxidation of methane to methanol over proton conductor/metal mixed catalysts**

pp 195–200

Byungik Lee, Yosuke Sakamoto, Daisuke Hirabayashi, Kenzi Suzuki, Takashi Hibino\*

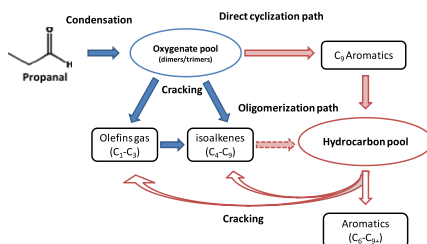


An electrochemical reactor for direct methanol synthesis from methane is downsized from macro- to micro- or nanoscale and operated without the need for an electrical power source.

**A comparison of the reactivities of propanal and propylene on HZSM-5**

pp 201–208

Trung Q. Hoang, Xinli Zhu, Tawan Sooknoi, Daniel E. Resasco, Richard G. Mallinson\*

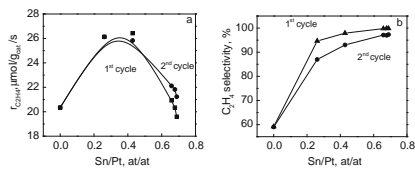


Propanal is found to be much more reactive than propylene and to form mostly 2-methyl-2-pentenal and C<sub>9</sub> aromatics as early products in the reaction network through the aldol pathway.

**Ethane dehydrogenation on Pt/Mg(Al)O and PtSn/Mg(Al)O catalysts**

pp 209–219

Vladimir Galvita, Georges Siddiqi, Pingping Sun, Alexis T. Bell\*

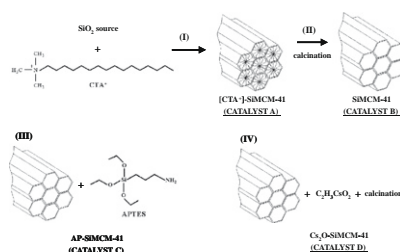


The effects of Sn on the dehydrogenation of ethane on Pt supported on calcined hydrotalcite (Pt/Mg(Al)O) were investigated. Sn was found to form an alloy with Pt and to enhance ethene selectivity and decrease coke deposition. Adsorption of ethene was identified as the primary source of CH<sub>x</sub> (x = 1–3) species that are precursors to the formation of methane and coke.

**Preparation of different basic Si–MCM-41 catalysts and application in the Knoevenagel and Claisen–Schmidt condensation reactions**

pp 220–227

Leandro Martins, Wolfgang Hölderich, Peter Hammer, Dilson Cardoso\*

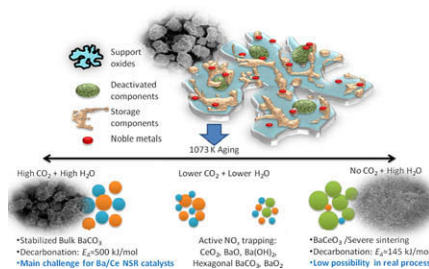


For the first time, the basicity of Si–MCM-41 mesoporous materials was compared with the as-synthesized material [CTA<sup>+</sup>]-Si–MCM-41 (CTA<sup>+</sup> stands for the structure directing agent).

**Effects of CO<sub>2</sub> and steam on Ba/Ce-based NO<sub>x</sub> storage reduction catalysts during lean aging**

pp 228–238

Ming Yang, Yuping Li, Jun Wang, Meiqing Shen\*

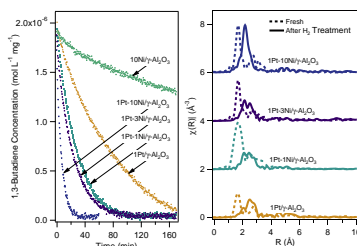


NO<sub>x</sub> storage/reduction catalysts based on barium and cerium oxides were treated under different aging atmospheres to reveal the effects of CO<sub>2</sub> and steam on the chemical and morphological properties of the materials.

**Correlating extent of Pt–Ni bond formation with low-temperature hydrogenation of benzene and 1,3-butadiene over supported Pt/Ni bimetallic catalysts**

pp 239–250

William W. Lonergan, Dionisios G. Vlachos, Jingguang G. Chen\*

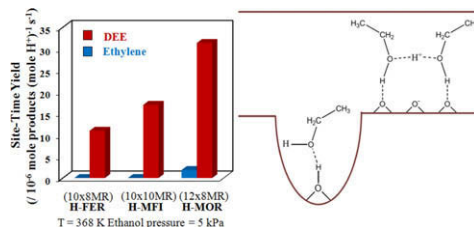


Hydrogenation activity was found to correlate to the extent of Pt–Ni bimetallic bond formation, as characterized by the coordination numbers obtained through EXAFS analysis of the Pt L<sub>III</sub>-edge.

## Catalytic consequences of hydroxyl group location on the rate and mechanism of parallel dehydration reactions of ethanol over acidic zeolites

pp 251–261

Hsu Chiang, Aditya Bhan\*

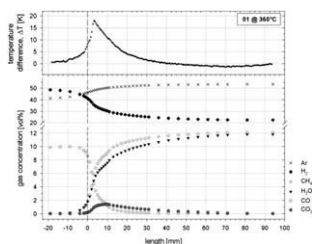


In zeolite pores large enough to accommodate ethanol dimers, ethanol preferentially dehydrates via a bimolecular pathway to generate diethyl ether since the formation of ethanol dimeric species is energetically more favorable than the formation of ethanol monomers. In zeolite channels too small to accommodate ethanol dimers, ethanol is selectively dehydrated via a unimolecular reaction pathway to generate ethylene.

## Applying spatially resolved concentration and temperature measurements in a catalytic plate reactor for the kinetic study of CO methanation

pp 262–279

Jan Kopyscinski, Tilman J. Schildhauer\*, Frédéric Vogel, Serge M.A. Biollaz, Alexander Wokaun

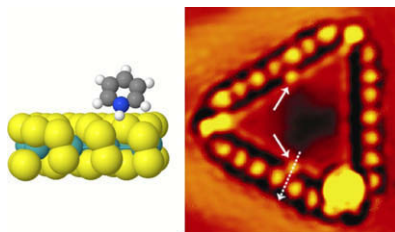


Spatially resolved gas concentration and catalyst temperature measurements in an optically accessible catalytic plate reactor allowed determining the kinetics of the exothermic CO methanation reaction with high initial CO partial pressure.

## Atomic-scale insight into the origin of pyridine inhibition of $\text{MoS}_2$ -based hydrotreating catalysts

pp 280–289

Burcin Temel, Anders K. Tuxen, Jakob Kibsgaard, Nan-Yu Topsøe, Berit Hinnemann\*, Kim G. Knudsen, Henrik Topsøe, Jeppe V. Lauritsen\*, Flemming Besenbacher

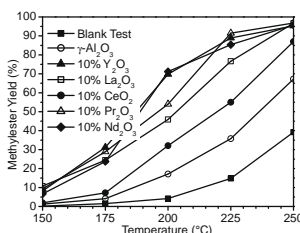


Inhibition of catalytic hydrodesulfurization activity is related to pyridinium species that are directly observed to adsorb strongly on the edges of  $\text{MoS}_2$  nanoclusters.

## New rare earth oxide catalysts for the transesterification of triglycerides with methanol resulting in biodiesel and pure glycerol

pp 290–304

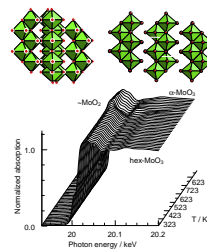
Bernhard M.E. Russbueltdt, Wolfgang F. Hoelderich\*



Pure rare earth oxides, supported rare earth oxides, and stoichiometric rare earth mixed oxide catalysts were used for the transesterification of different oils and fats with methanol. Structure–activity relationships are depicted.

**Structure and properties of a Mo oxide catalyst supported on hollow carbon nanofibers in selective propene oxidation** pp 305–314

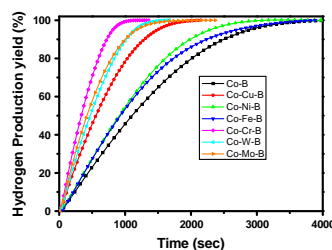
T. Ressler\*, A. Walter, J. Scholz, J.-P. Tessonnier, D.S. Su



Molybdenum oxide supported on hollow vapor-grown carbon nanofibers is active in oxidation of propene to acrylic acid. In situ XAS under reaction conditions showed structural transformation from hex-MoO<sub>3</sub> to  $\alpha$ -MoO<sub>3</sub>.

**Promoting effect of transition metal-doped Co–B alloy catalysts for hydrogen production by hydrolysis of alkaline NaBH<sub>4</sub> solution** pp 315–324

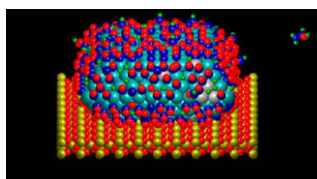
N. Patel\*, R. Fernandes, A. Miotello



Cr-, W-, Mo-, and Cu-doped Co–B catalyst showed 3–4 times increment in H<sub>2</sub> generation rate when compared to the undoped catalyst for hydrolysis of NaBH<sub>4</sub> at 298 K, while Ni and Fe are only able to create a marginal increment in the catalytic performance.

**Ethanol synthesis from syngas over Rh-based/SiO<sub>2</sub> catalysts: A combined experimental and theoretical modeling study** pp 325–342

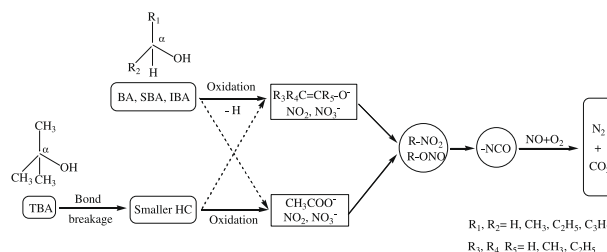
Donghai Mei\*, Roger Rousseau, Shawn M. Kathmann, Vassiliki-Alexandra Glezakou, Mark H. Engelhard, Weilin Jiang, Chongmin Wang, Mark A. Gerber, James F. White, Don J. Stevens



Combining experimental measurements with first-principles-based kinetic Monte Carlo modeling, the reaction kinetics of ethanol synthesis from CO hydrogenation over Rh/Mn/SiO<sub>2</sub> catalysts was studied. We find that addition of Mn promoter into Rh-based catalysts can lower CO insertion barriers thus improving the selectivity toward ethanol and other C<sub>2</sub> oxygenates. The effects of various promoters (M = Ir, Ga, V, Ti, Sc, Ca, and Li) on CO insertion step over Rh/M alloy nanoparticles were further investigated, suggesting that alloying the promoter with the electronegativity difference,  $\Delta\chi = 0.7$ , between the promoter M and Rh is the most effective in lowering CO insertion barriers which leads to higher selectivity to ethanol.

**Remarkable influence of reductant structure on the activity of alumina-supported silver catalyst for the selective catalytic reduction of NOx** pp 343–350

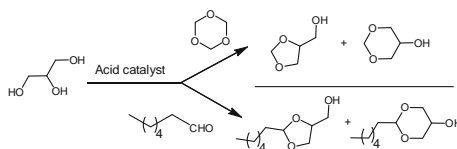
Yunbo Yu, Xiaoping Song, Hong He\*



The presence of  $\alpha$ -H is prerequisite for enolic species formation during NOx reduction by C<sub>4</sub> alcohols over Ag/Al<sub>2</sub>O<sub>3</sub>, playing a crucial role in the efficiency for NOx conversion.

## Gold catalysts and solid catalysts for biomass transformations: Valorization of glycerol and glycerol–water mixtures through formation of cyclic acetals pp 351–357

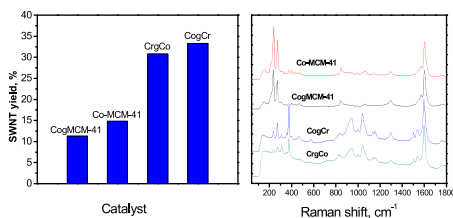
Violeta R. Ruiz, Alexandra Velty, Laura L. Santos, Antonio Leyva-Pérez, María J. Sabater, Sara Iborra, Avelino Corma\*



Gold salts and complexes are superior catalysts than other homo- and heterogeneous Brønsted and Lewis acids for obtaining valuable acetals from glycerol.

## A novel synthesis route for bimetallic CoCr–MCM-41 catalysts with higher metal loadings. Their application in the high yield, selective synthesis of Single-Wall Carbon Nanotubes pp 358–369

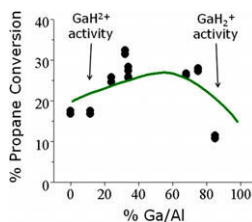
Codruta Zoican Loebick, Sungchul Lee, Salim Derrouiche, Mark Schwab, Yuan Chen, Gary L. Haller, Lisa Pfefferle\*



Characterization of SWNT synthesized on various catalytic systems: Co grafted on MCM-41 (CogMCM-41), Co incorporated on MCM-41 (Co–MCM-41), Cr grafted on Co–MCM-41 (CrgCo) and Co grafted on Cr–MCM-41 (CogCr). Left – resultant SWNT yield. Right – Resonant Raman Spectroscopy of SWNT.

## Identity and chemical function of gallium species inferred from microkinetic modeling studies of propane aromatization over Ga/HZSM-5 catalysts pp 370–385

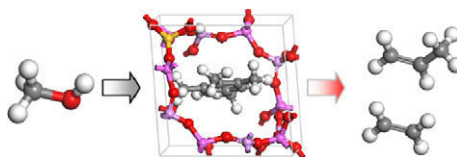
Gowri Krishnamurthy, Aditya Bhan, W. Nicholas Delgass\*



Unified gallium monohydride–gallium dihydride model predictions, indicating the regions where each active site dominates. All aluminum assumed to be in pairs, Si/Al = 16,  $T = 520$  °C, space time =  $1.514$  g<sub>cat</sub> h/mol.

## Catalytic activity and selectivity of methylbenzenes in HSAPO-34 catalyst for the methanol-to-olefins conversion from first principles pp 386–391

Chuan-Ming Wang, Yang-Dong Wang, Hong-Xing Liu, Zai-Ku Xie\*, Zhi-Pan Liu\*\*

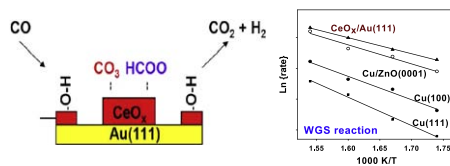


Theoretical calculations on the methanol-to-olefins conversion in HSAPO-34 reveal that hexamethylbenzene and pentamethylbenzene are not more active than methylbenzenes with fewer methyl groups, and propene is the favored product.

**Probing the reaction intermediates for the water–gas shift over inverse CeO<sub>x</sub>/Au(1 1 1) catalysts**

pp 392–400

Sanjaya D. Senanayake, Dario Stacchiola, Jaime Evans, Michael Estrella, Laura Barrio, Manuel Pérez, Jan Hrbek, José A. Rodriguez\*

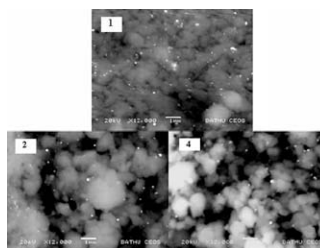


Water–gas shift reaction over an inverse CeO<sub>x</sub>/Au(1 1 1) catalyst: activity and relative stability of possible reaction intermediates (HO, HCOO and CO<sub>3</sub>).

**Deactivation of PtH-MFI bifunctional catalysts by coke formation during benzene alkylation with ethane**

pp 401–412

Li Min Chua, Tanya Vazhnova, Timothy J. Mays, Dmitry B. Lukyanov, Sean P. Rigby\*

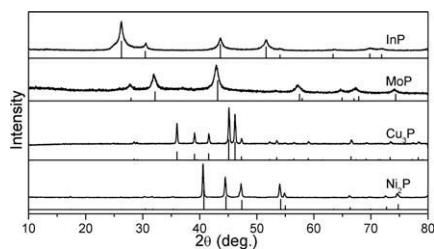


Backscattered scanning electron microscopy images of PtH-MFI-40 catalysts: Fresh (1), 4 h (2), and 48 h (4) on-stream.

**RESEARCH NOTE****A novel synthetic approach to synthesizing bulk and supported metal phosphides**

pp 413–415

Qingxin Guan, Wei Li\*



This approach uses metal oxide as precursors. Both bulk metal phosphides with special morphology and supported metal phosphides that are used as catalysts can be synthesized by this synthetic approach.