

# Abstracts

## CATALYSIS – APPLIED AND PHYSICAL ASPECTS

### Why is Metallic Pt the Best Catalyst for Methoxy Decomposition?

R. Ren, C. Niu, S. Bu, Y. Zhou, Y. Lv and G. Wang, *J. Nat. Gas Chem.*, 2011, **20**, (1), 90–98

The decomposition of methoxy on Cu(111), Ag(111), Au(111), Ni(111), Pt(111), Pd(111) and Rh(111) has been analysed by DFT calculations. The calculated activation barriers were correlated with the coupling matrix element  $V_{ad}^2$  and the  $d$ -band center ( $\epsilon_d$ ) for the Group IB metals and Group VIII metals, respectively. By comparison of the activation energy barriers of the methoxy decomposition, Pt was found to be the best catalyst.

### The Atomic Structural Dynamics of $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Supported Ir–Pt Nanocluster Catalysts Prepared from a Bimetallic Molecular Precursor: A Study Using Aberration-Corrected Electron Microscopy and X-Ray Absorption Spectroscopy

M. W. Small, S. I. Sanchez, L. D. Menard, J. H. Kang, A. I. Frenkel and R. G. Nuzzo, *J. Am. Chem. Soc.*, 2011, **133**, (10), 3582–3591

Deposition of [Ir<sub>3</sub>Pt<sub>3</sub>( $\mu$ -CO)<sub>3</sub>(CO)<sub>3</sub>( $\eta$ -C<sub>5</sub>Me<sub>5</sub>)<sub>3</sub>] on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, and its subsequent reduction with H<sub>2</sub>, gave highly dispersed supported bimetallic Ir–Pt NPs. Various characterisation techniques were combined to show that Ir–Pt NPs supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> containing a 1:1 ratio of Ir:Pt adopt segregated structures in which Ir occupies the core region.

### Kinetics and Product Distribution Studies on Ruthenium-Promoted Cobalt/Alumina Fischer-Tropsch Synthesis Catalyst

A. Tavasoli, A. Nakhaei Pour and M. G. Ahangari, *J. Nat. Gas Chem.*, 2010, **19**, (6), 653–659

HC production rates and distributions on Ru promoted Al<sub>2</sub>O<sub>3</sub> supported Co Fischer-Tropsch synthesis catalyst were investigated by the concept of two superimposed Anderson-Schulz-Flory (ASF) distributions. The characterising growth probabilities  $\alpha_1$  and  $\alpha_2$  are strongly dependent on reaction conditions. By increasing the H<sub>2</sub>/CO partial pressure ratios and reaction temperatures, deviation from normal ASF distribution decreases and the double- $\alpha$ -ASF distribution changes into a straight line. Based on the concept of double- $\alpha$ -ASF distribution, a rate equation for the production of HCs was obtained.

## CATALYSIS – REACTIONS

### Catalytic Oxidation of Biomass Tar over Platinum and Ruthenium Catalysts

S. J. Yoon, Y. K. Kim and J. G. Lee, *Ind. Eng. Chem. Res.*, 2011, **50**, (4), 2445–2451

The catalytic oxidation of toluene was investigated using Pt and Ru on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. As the reaction temperature increased and the size of the catalyst decreased, the conversion of toluene increased. Usually, the higher content of Pt and Ru showed higher conversion of toluene. The Pt catalyst showed a higher toluene conversion efficiency than the Ru catalyst at the same temperature in the absence of syngas; while in the presence of syngas, the Ru catalyst showed a better conversion efficiency than the Pt catalyst. A temperature of >300°C is required to oxidise tar efficiently.

## EMISSIONS CONTROL

### Effect of Palladium Dispersion on the Capture of Toxic Components from Fuel Gas by Palladium-Alumina Sorbents

J. P. Baltrus, E. J. Granite, E. C. Rupp, D. C. Stanko, B. Howard and H. W. Pennline, *Fuel*, 2011, **90**, (5), 1992–1998

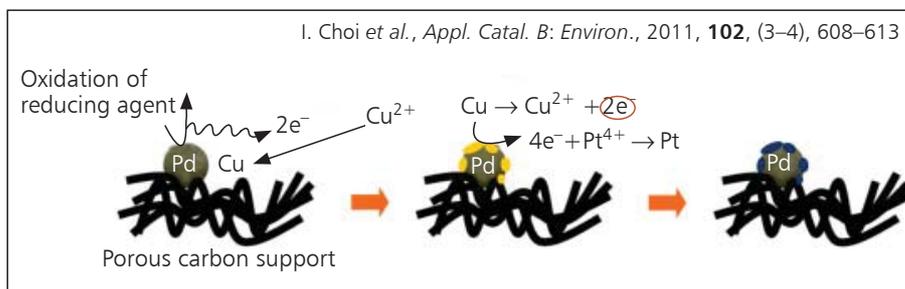
The preparation method used for Pd/Al<sub>2</sub>O<sub>3</sub> sorbents was found to influence their performance. When Pd is well dispersed in the pores of the support, Pd is less susceptible to S poisoning, and the sorbent has better long-term activity for adsorption of AsH<sub>3</sub> and H<sub>2</sub>Se, but poorer adsorption capacity for Hg. As the contact interaction between Pd and the support is lessened the Pd becomes more susceptible to poisoning by S, resulting in higher capacity for Hg, but poorer long-term performance for adsorption of As and Se.

## FUEL CELLS

### Preparation of Pt<sub>shell</sub>–Pd<sub>core</sub> Nanoparticle with Electroless Deposition of Copper for Polymer Electrolyte Membrane Fuel Cell

I. Choi, S. H. Ahn, J. J. Kim and O. J. Kwon, *Appl. Catal. B: Environ.*, 2011, **102**, (3–4), 608–613

The title NP was prepared by an electrochemical method (see the figure). Pd/C was surrounded by Cu through electroless deposition which was followed by a displacement reaction with Pt. The catalytic properties



were investigated using RDE. The kinetics of the electrochemically-prepared Pt/Pd/C catalyst for  $O_2$  reduction were superior to a conventional Pt/C catalyst. The Pt<sub>shell</sub>-Pd<sub>core</sub> NP contains small amount of Pt leading to high mass-specific activity.

#### Palladium-Based Electrodes: A Way to Reduce Platinum Content in Polymer Electrolyte Membrane Fuel Cells

E. Antolini, S. C. Zignani, S. F. Santos and E. R. Gonzalez, *Electrochim. Acta*, 2011, **56**, (5), 2299–2305

A Pd-based PEMFC was formed using a Pd<sub>96</sub>Pt<sub>4</sub>/C anode catalyst and a Pd<sub>49</sub>Pt<sub>47</sub>Co<sub>4</sub>/C cathode catalyst. When the overall Pd:Pt:Co atomic composition of both electrodes (anode + cathode) was 72:26:2, the cell performance at a current density of 1 A cm<sup>-2</sup> was 89% that of a conventional Pt/C-catalysed PEMFC. Of the performance loss, 6% was ascribed to the anode catalyst and 5% to the cathode catalyst. The performance losses were thought to be due to the higher particle size of the Pd-based catalysts compared to Pt. The maximum power density of the Pd-based cell was 76% of that of a Pt/C-catalysed cell.

#### Rapid Optical Screening Technology for Direct Methanol Fuel Cell (DMFC) Anode and Related Electrocatalysts

F. G. Welsch, K. Stöwe and W. F. Maier, *Catal. Today*, 2011, **159**, (1), 108–119

An optical high-throughput screening method for DMFC catalysts based on the fluorescence of protonated quinine generated during electrooxidation of MeOH has been developed. The working electrode allows the parallel quantification of the fluorescence development for up to 60 materials. For the preparation of the working electrode a coating routine was employed, which allows the use of sol-gel derived materials. Due to the required stability of the electrode catalysts towards the acidic polymer membrane, a fast optical prescreening method for acid stable materials was

developed. The method was validated with Pt-Ru electrocatalysts.

## METALLURGY AND MATERIALS

#### Stress Induced Deformation in the Solidification of Undercooled Co<sub>80</sub>Pd<sub>20</sub> Alloys

S. Zhou, R. Hu, J. Li, H. Chang, H. Kou and L. Zhou, *Mater. Sci. Eng.: A*, 2011, **528**, (3), 973–977

The Co<sub>80</sub>Pd<sub>20</sub> alloys were undercooled by denucleation of molten glasses combined with cyclic superheating. The highest undercooling achieved was 415 K. Dense-regular fault ribbons were detected in high undercooling grains of Co<sub>80</sub>Pd<sub>20</sub>. It provided experimental evidence of stress existed in solidification process at high undercooling.

#### The Effect of Fe Additions on the Shape Memory Properties of Ru-Based Alloys

A. Manzoni, K. Chastaing, A. Denquin, P. Vermaut, J. van Humbeeck and R. Portier, *Scripta Mater.*, 2011, **64**, (12), 1071–1074

Equiatomic RuNb and RuTa shape memory alloys exhibit a shape memory effect (SME) and transformation temperatures >800°C. Controlling the transformation temperatures while retaining the SME could be achieved either by changing the alloy composition or by adding a ternary element such as Fe. Eight alloys were investigated and compression testing and DSC were carried out. The SME was found to decrease with decreasing Ru content.

## APPARATUS AND TECHNIQUE

#### Acetylene Sensor Based on Pt/ZnO Thick Films as Prepared by Flame Spray Pyrolysis

N. Tamaekong, C. Liewhiran, A. Wisitsoraat and S. Phanichphant, *Sens. Actuators B: Chem.*, 2011, **152**, (2), 155–161

ZnO nanoparticles loaded with Pt were produced by flame spray pyrolysis using Zn naphthenate

and Pt(II) acetylacetonate precursors dissolved in xylene. Under the 5/5 (precursor/oxygen) flame condition, ZnO nanoparticles and nanorods were obtained. The crystallite sizes of ZnO spherical and hexagonal particles were from 5 to 20 nm while ZnO nanorods were 5–20 nm in width and 20–40 nm in length. Pt NPs with diameter of ~1 nm were uniformly deposited on the surface of ZnO particles. Acetylene sensing characteristics of ZnO NPs was significantly improved as Pt content increased from 0 to 2 at%. A low detection limit of 50 ppm was obtained at 300°C operating temperature.

#### TG/DTA of Hydrogen Reduction Kinetics of TiO<sub>2</sub> Supported PdO Chemoschromic Pigments

N. Mohajeri, A. T-Raissi and J. Baik, *Thermochim. Acta*, 2011, **518**, (1–2), 119–122

TiO<sub>2</sub>-supported PdO chemochromic pigments were used in H<sub>2</sub> sensing devices for detecting H<sub>2</sub> leaks. TG/DTA analysis was used to study the kinetics of reduction of PdO/TiO<sub>2</sub> by H<sub>2</sub> gas and revealed a two-step process. A colour change was associated with the second step during which the adsorbed H<sub>2</sub> reacts with PdOH species to form water. This step has fast kinetics with reaction order of 0.55 and zero with respect to [PdOH] and [H<sub>2</sub>], respectively.

## ELECTROCHEMISTRY

#### Molecular Adsorbates at Single-Crystal Platinum-Group Metals and Bimetallic Surfaces

H. Baltruschat and S. Ernst, *ChemPhysChem*, 2011, **12**, (1), 56–69

Fundamental studies of the molecule–surface interaction between organic species such as CO, C<sub>6</sub>H<sub>6</sub> and C<sub>2</sub>H<sub>2</sub> and Pt, Pd or their (sub)monolayers on Au are reviewed. The surface orientation of the pgms was found to determine the kind of organic species that would adsorb on them as well as the prevailing reaction channels. Pd was less active than Pt for oxidation or hydrogenation of the adsorbates. The experimental results are of interest as models for more complicated adsorbates in the context of electrochemical sensors, electroorganic synthesis, corrosion inhibitors and brighteners for metal plating as well as electrocatalytic processes. (Contains 107 references.)

## PHOTOCONVERSION

#### Photooxidation of 1,5-Dihydroxynaphthalene with Iridium Complexes as Singlet Oxygen Sensitizers

S. Takizawa, R. Aboshi and S. Murata, *Photochem. Photobiol. Sci.*, 2011, **10**, (6), 895–903

Photooxidation of 1,5-dihydroxynaphthalene was carried out in the presence of cyclometallated neutral and cationic Ir complexes as singlet oxygen (<sup>1</sup>O<sub>2</sub>) sensitizers. [Ir(ppy)<sub>2</sub>(phen)]<sup>+</sup> and [Ir(ppy)<sub>2</sub>(bpy)]<sup>+</sup> have high <sup>1</sup>O<sub>2</sub> generation quantum yields. The neutral complexes with lower oxidation potentials were considered to have a more efficient charge-transfer interaction with molecular oxygen, which decreased the efficiency of <sup>1</sup>O<sub>2</sub> formation. High yields of the oxidised product when using the cationic complexes indicated their excellent photosensitising durability.

#### A Phosphorescent Material with High and Balanced Carrier Mobility for Efficient OLEDs

T. Peng, Y. Yang, Y. Liu, D. Ma, Z. Hou and Y. Wang, *Chem. Commun.*, 2011, **47**, (11), 3150–3152

A novel phosphorescent material (Fppy)<sub>2</sub>Ir(dipba) was shown to possess superior hole and electron transporting properties. (Fppy)<sub>2</sub>Ir(dipba) performed as an efficient phosphorescent emitter as well as an excellent host for a yellow phosphorescent dopant to result in high-performance PHOLEDs. The results suggest that electroluminescence performance of PHOLEDs based on doping strategy can be enhanced by using the phosphorescent complexes with the improved charge carrier transporting property as the host.

## SURFACE COATINGS

#### Electrodeposition of Al–Pt Alloys Using Constant Potential Electrolysis in AlCl<sub>3</sub>–NaCl–KCl Molten Salt Containing PtCl<sub>2</sub>

M. Ueda, H. Hayashi and T. Ohtsuka, *Surf. Coat. Technol.*, 2011, **205**, (19), 4401–4403

Molten salt electrolysis with an AlCl<sub>3</sub>–NaCl–KCl molten salt containing PtCl<sub>2</sub> at 448 K was used to form Al–Pt alloys for high-temperature coatings. The voltammogram showed that cathodic reduction of Pt ions started at a potential of 1.4 vs. Al/Al(III) in the molten salt. Pure Pt was deposited at 1.2 V and there was co-deposition of Al and Pt at potentials <1.0 V. The co-deposit was a mixture of intermetallic compounds of AlPt<sub>2</sub> or AlPt<sub>3</sub>. The ratio of Pt:Al (in at%) in the electrodeposits decreased from 100:0 at 1.2 V to 25:75 at 0.0 V.