

Abstracts

CATALYSIS – APPLIED AND PHYSICAL ASPECTS

Terminal $\text{C}\equiv\text{C}$ Triple Bond Hydrogenation Using Immobilized Wilkinson's Catalyst

E. Leitmannová, P. Jirásek, J. Rak, L. Potucká, P. Kačer and L. Červený, *Res. Chem. Intermed.*, 2010, **36**, (5), 511–522

Phenylacetylene was selectively hydrogenated to styrene and 3-phenylpropyne to allylbenzene using Wilkinson's catalyst immobilised by ionic exchange on hectorite and montmorillonite or by covalent bonding on MCM-41 and SBA-15. Heterogeneous catalysis was more selective than homogeneous catalysis for phenylacetylene hydrogenation. The type of immobilisation had no influence on activity or selectivity.

Osmium(III) Complexes with POP Pincer Ligands: Preparation from Commercially Available $\text{OsCl}_3\cdot 3\text{H}_2\text{O}$ and Their X-ray Structures

G. Asensio, A. B. Cuenca, M. A. Esteruelas, M. Medio-Simón, M. Oliván and M. Valencia, *Inorg. Chem.*, 2010, **49**, (19), 8665–8667

Os complexes with phosphine ligands such as $\text{dbf}(\text{P}^i\text{Pr}_2)_2$, $\text{xant}(\text{P}^i\text{Pr}_2)_2$ or $\text{xant}(\text{PPh}_2)_2$ were obtained in high yields by reaction of the corresponding diphosphine with $\text{OsCl}_3\cdot 3\text{H}_2\text{O}$. The corresponding Ru(III) complexes were similarly obtained from $\text{RuCl}_3\cdot 3\text{H}_2\text{O}$ in moderate yields. The X-ray structures of $\text{dbf}(\text{P}^i\text{Pr}_2)_2$ and the synthesised Os complexes are also reported.

Synthesis and RCM Reactions Using a Recyclable Grubbs–Hoveyda Metathesis Catalyst Activated by a Light Fluorous Tag

M. Matsugi, Y. Kobayashi, N. Suzumura, Y. Tsuchiya and T. Shioiri, *J. Org. Chem.*, 2010, **75**, 22, 7905–7908

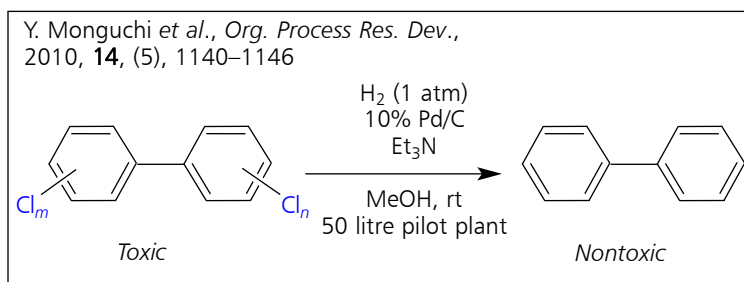
A recyclable Grubbs–Hoveyda second-generation catalyst activated by a light fluorous tag was prepared. The catalyst exhibited higher activity than the parent or a previously reported variant for RCM reactions and could be routinely recovered. The light fluorous tag in the catalyst served as both an activator and a handle for separation and recovery by fluorous solid-phase extraction.

CATALYSIS – INDUSTRIAL PROCESS

Pilot-Plant Study of the PCB Degradation at Ambient Temperature and Pressure

Y. Monguchi, S. Ishihara, A. Ido, M. Niikawa, K. Kamiya, Y. Sawama, H. Nagase and H. Sajiki, *Org. Process Res. Dev.*, 2010, **14**, (5), 1140–1146

A continuous pilot plant for the degradation of polychlorinated biphenyls (PCBs) by Pd/C-catalysed hydrogenation in the presence of NEt_3 (see the Figure) was designed and constructed. Undiluted PCBs from a capacitor and diluted PCBs with desulfurised trans oil could be decomposed at ambient temperature and pressure. This degradation method can be combined with catalytic desulfurisation technology for the purification of gasoline and kerosene.



EMISSIONS CONTROL

Loading and Aging Effects in Exhaust Gas After-Treatment Catalysts with Pt as Active Component

W. Boll, S. Tischer and O. Deutschmann, *Ind. Eng. Chem. Res.*, 2010, **49**, (21), 10303–10310

Several close-to-production DOCs with Pt loadings between $22\text{--}130\text{ g ft}^{-3}$ were hydrothermally aged between $700\text{--}950^\circ\text{C}$ and characterised by BET, HR-SEM, HR-TEM and CO-TPD. The pollutant conversion could be predicted for DOCs and NSCs with different Pt loadings and under different ageing conditions by determining the catalytically active surface area using CO-TPD.

Simulation of a Nonisothermal Modern Three-Way Catalyst Converter

H. J. Kwon, J. H. Baik, S. B. Kang, I.-S. Nam, B. J. Yoon and S. H. Oh, *Ind. Eng. Chem. Res.*, 2010, **49**, (15), 7039–7051

A 2D nonisothermal monolith reactor model based on intrinsic detailed reaction kinetics was developed to simulate the performance of a commercial TWC.

The model predicts TWC performance for both Pd (front) and Pt/Rh/Ce (rear) monolith bricks. The reactor model was further validated by predicting the TWC performance of the dual-bed reactor under the steady-state sweep test (st-ST) condition varying the air:fuel ratios from 14.23 to 15.03 at different reaction temperatures.

FUEL CELLS

A One-Step Continuous Synthesis of Carbon-Supported Pt Catalysts Using a Flame for the Preparation of the Fuel Electrode

I. D. Choi, H. Lee, Y.-B. Shim and D. Lee, *Langmuir*, 2010, **26**, (13), 11212–11216

A single-step method for continuous production of up to 60 wt% Pt/C catalysts for the fuel electrode of a PEMFC is reported. An acetylene-air diffusion flame was used as the source of both heat and C, and Pt(acac)₂-containing xylene droplets were injected into the flame. Size was controlled at 2–7 nm. The electrochemical activity was >74.9 m² g⁻¹ Pt, more efficient than an equivalent commercial (E-TEK 10 wt% Pt) catalyst.

Improvement of Platinum Adhesion to Carbon Surfaces Using PVD Coatings

M. Shafiei, A. R. Riahi, F. G. Sen and A. T. Alpas, *Surf. Coat. Technol.*, 2010, **205**, (2), 306–311

Adhesion of Pt to modified C surfaces was assessed experimentally using a micro scratch test, and the bond strengths were calculated by first principles simulations. Pt adhesion to graphite could be improved by applying thin interfacial layers of Au, Ti or Cr, which may enhance the Pt catalyst durability in PEMFCs. Pt adhesion to non-hydrogenated diamond-like C was strong enough without the application of these thin layers.

Colloidal Synthesis and Characterization of Carbon-Supported Pd–Cu Nanoparticle Oxygen Reduction Electrocatalysts

N. N. Kariuki, X. Wang, J. R. Mawdsley, M. S. Ferrandon, S. G. Niyogi, J. T. Vaughey and D. J. Myers, *Chem. Mater.*, 2010, **22**, (14), 4144–4152

Colloidal synthesis was used to prepare monodisperse Pd-Cu alloy nanoparticles with average diameter 3 nm for the as-prepared particles and 5–10 nm after removal of the capping agents. The resulting nanoparticles were deposited on high surface area C

to form Pd-Cu/C catalysts. Their ORR activity in acidic electrolyte was high and depended on composition and heat treatment conditions.

METALLURGY AND MATERIALS

Effect of Modification by Pt and Manufacturing Processes on the Microstructure of Two NiCoCrAlYTa Bond Coatings Intended for Thermal Barrier System Applications

A. Vande Put, M.-C. Lafont, D. Oquab, A. Raffaitin and D. Monceau, *Surf. Coat. Technol.*, 2010, **205**, (3), 717–727

Pt was added to two NiCoCrAlYTa coatings made by different manufacturing processes. XRD, SEM, EDS and TEM analyses showed that the Pt layer caused Al uphill diffusion from the NiCoCrAlYTa bulk to the Pt-rich surface during heat treatment. This is expected to provide good oxidation and hot corrosion resistance. The final microstructure was also influenced by the manufacturing process.

ELECTROCHEMISTRY

Observing Iridium Oxide (IrO_x) Single Nanoparticle Collisions at Ultramicroelectrodes

S. J. Kwon, F.-R. F. Fan and A. J. Bard, *J. Am. Chem. Soc.*, 2010, **132**, (38), 13165–13167

The electrochemical detection of single IrO_x nanoparticle collisions on a NaBH₄-treated Pt ultramicroelectrode (UME) was carried out for the electrocatalytic water oxidation reaction. IrO_x transiently sticks to the electrode, causing a reversible 'spike' in the current. The frequency of spikes was directly proportional to particle concentration, and the peak current increased with applied potential. The observed current was sensitive to the material and surface state of the measuring electrode; a NaBH₄-treated Pt UME was important for reproducibility.

NANOTECHNOLOGY

Shape Control of Platinum and Palladium Nanoparticles for Catalysis

S. Cheong, J. D. Watt and R. D. Tilley, *Nanoscale*, 2010, **2**, (10), 2045–2053

This mini review surveys solution-phase methods for preparing shaped Pt and Pd nanoparticles with specific crystallographic facets. Catalytic studies of the shaped nanoparticles and results of their activity and

selectivity are highlighted. Aspects of synthesis and catalysis to be considered for the future development of more efficient and effective catalysts are given. (Contains 94 references.)

Electrochemical Pd Nanodeposits on a Au Nanoisland Template Supported on Si(100): Formation of Pd–Au Alloy and Interfacial Electronic Structures

Y. Sohn, D. Pradhan and K. T. Leung, *ACS Nano*, 2010, **4**, (9), 5111–5120

Pd nanoparticles (Pd NPs) were electrodeposited on a H-terminated Si(100) substrate and on a Au nanoisland template (NIT) supported on Si(100). As-deposited Pd NPs on H:Si consisted primarily of a metallic Pd core with Pd_xSi at the Pd and Si interface. Annealing the Pd NPs to 700°C in air promoted formation of PdO with an overlayer of PdO₂. Pd NPs on supported Au NIT formed a Pd–Au alloy at room temperature at the metallic Pd and Au nanoisland interface. This was further enhanced by post-annealing at 700°C.

PHOTOCONVERSION

Red-Phosphorescent OLEDs Employing Iridium (III) Complexes Based on 5-Benzoyl-2-phenylpyridine Derivatives

K. H. Lee, H. J. Kang, J. K. Park, J. H. Seo, Y. K. Kim and S. S. Yoon, *Thin Solid Films*, 2010, **518**, (22), 6188–6194

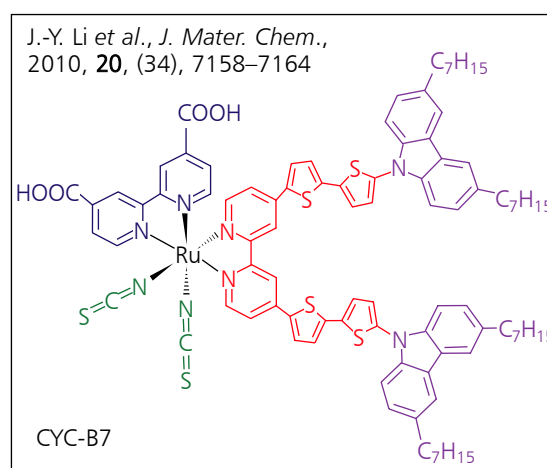
Proceedings of the 2nd International Conference on Microelectronics and Plasma Technology – ICMAP 2009

A series of red phosphorescent Ir(III) complexes based on 5-benzoyl-2-phenylpyridine derivatives was synthesised. Their photophysical and electrophosphorescent properties were investigated. Multilayered OLEDs with efficient red emissions were fabricated. The maximum luminance was 14,200 cd m⁻² at 14.0 V. Luminous, power, and quantum efficiency were 10.40 cd A⁻¹, 3.44 lm W⁻¹ and 9.21% at 20 mA cm⁻², respectively. The peak electroluminescence wavelength was 607 nm, with CIE coordinates of (0.615, 0.383) at 12.0 V. The device also showed a stable colour chromaticity with various voltages.

Heteroleptic Ruthenium Antenna-Dye for High-Voltage Dye-Sensitized Solar Cells

J.-Y. Li, C.-Y. Chen, J.-G. Chen, C.-J. Tan, K.-M. Lee, S.-J. Wu, Y.-L. Tung, H.-H. Tsai, K.-C. Ho and C.-G. Wu, *J. Mater. Chem.*, 2010, **20**, (34), 7158–7164

A new Ru photosensitiser, CYC-B7 (see the **Figure**), with an electron-rich bithiophene and a bis-heptyl-substituted carbazole substituent was found to increase the open-circuit voltage (V_{oc}) of a dye-sensitised solar cell (DSSC) device to 788 mV, with an overall conversion efficiency (η) of 8.96%. The MLCT transition band was centred at 551 nm and the molar absorption coefficient was $2.19 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$.



SURFACE COATINGS

Atomic Layer Deposition of Ru/RuO₂ Thin Films Studied by *In Situ* Infrared Spectroscopy

S. K. Park, R. Kanjolia, J. Anthis, R. Odedra, N. Boag, L. Wielunski and Y. J. Chabal, *Chem. Mater.*, 2010, **22**, (17), 4867–4878

Ru(Cp)(CO)₂Et and O_{2(g)} were used as reactants for the deposition of Ru thin films. Sample temperature, precursor pulse length and precursor gas pressure were varied to achieve self-terminated surface reactions on H-terminated Si(111) surfaces. Higher growth rates (~1.5–3 Å/cycle) were obtained compared to those typical of ALD of metals (~0.5–1 Å/cycle) under saturation conditions. The deposition rate was linear and the film became metallic after 22 cycles. Thick films (45 nm) grown with short pulses produced metallic polycrystalline Ru with hcp structure.