

**Cover**

Image provided courtesy of computational science company Accelrys (www.accelrys.com). An electron density isosurface mapped with the electrostatic potential for an organometallic molecule. This shows the charge distribution across the surface of the molecule with the red area showing the positive charge associated with the central metal atom. Research carried out using Accelrys' Materials Studio[®].

Preface

7

James J. Spivey and Kerry M. Dooley**

Heterogeneous catalysis for production of value-added chemicals from biomass

13

*Kresten Egeblad, Jeppe Rass-Hansen, Charlotte C. Marsden, Esben Taarning and Claus Hviid Christensen**

Introduction	13
Setting a new scene	14
Catalytic C–C bond breaking	17
Catalytic hydrolysis	23
Catalytic dehydrations	25
Catalytic oxidations	32
Catalytic hydrogenations	39
Summary and outlook	43

Catalytic and photocatalytic removal of pollutants from aqueous sources

51

J. A. Anderson and M. Fernández-García*

General introduction	51
Catalytic elimination of inorganics	53
Photocatalytic removal of inorganics	60
Catalytic and photocatalytic removal of organometallics	65
Catalytic and photocatalytic removal of organics	65
Removal of microorganisms	73

Nano-architecture and reactivity of titania catalytic materials.	82
Part 2. Bidimensional nanostructured films	
<i>Gabriele Centi and Siglinda Perathoner</i>	
Introduction	82
Outlooks for the development of catalysts based on the concept of nanostructured films	89
Synthesis of titania nanostructured films	100
Uses, with focus on catalysis	106
Conclusions	119
<hr/>	
Recent advances in heterogeneous catalysis enabled by first-principles methods	131
<i>Ye Xu</i>	
Introduction	131
Theory-aided catalyst design	133
Molecular-level effects of reaction environment	137
Outlook	146
<hr/>	
Ionic liquids as catalysts, solvents and conversion agents	154
<i>Amit C. Gujar and Mark G. White</i>	
Introduction	154
Solubility of substrates in ionic liquids	155
Physical and chemical properties of ionic liquids	156
Demonstration of utility of RTILs as reaction solvents	157
Review articles	157
Synthesis of aluminum-containing ILs	158
Alkoxy carbonylation	159
Arene carbonylation	159
Catalytic oxidations	162
Diels–Alder reactions in ILs	162
Dimerization of olefins in ILs	164
Enzyme-catalyzed reactions	165
Fischer esterifications in ILs	166
Friedel–Crafts reactions in ILs	166
Heck reaction	169
Henry reactions in ILs	170
Hydrogenation in ILs	171
Hydroformylation	173
Isomerization	176
Metathesis of olefins	177
Michael reaction	177
Pechmann condensation in ILs	179
Sonogashira reaction	179
Sulfonation of arenes	181

Supported analogs of ionic liquid catalysts	181
Task specific ionic liquids (TSIL)	182
Telomerization in ILs	184

**Measurement techniques in catalysis for mechanism development:
kinetic, transient and *in situ* methods** 191

Nora M. McLaughlin and Marco J. Castaldi

Introduction	191
Structure to kinetics	192
Surface measurement techniques	193
Current <i>in situ</i> measurement techniques	197
Future directions	215

