

Development of new catalyst-solvent systems for liquid phase heterogeneously catalysed reactions

Christopher Hardacre

School of Chemistry and Chemical Engineering/CenTACat,
Queen's University, Belfast, BT9 5AG, UK

E-mail: c.hardacre@qub.ac.uk

Abstract

This presentation will examine the use of density functional theory to understand and predict new catalysts for the hydrogenation of amides to form amines at low pressures and temperatures. The catalysts developed were also examined for the hydrogenation of carboxylic acids to form both alkanes and alcohols. From the DFT it is clear that monometallic catalysts are not suitable for amide hydrogenation and bimetallic systems are required in order to activate the carbon-oxygen bond as well as reduce the atomic oxygen produced to form water and regenerate the catalyst. Acid hydrogenation is possible with monometallic catalysts and, in fact, these catalysts are more selective for alcohol formation compared with the bimetallic catalysts which predominantly form alkanes. The DFT has provided the basis for the newly developed catalysts which have been optimised using experimental methods to form materials which are active below 100 °C and 20 bar. In addition, the presentation will discuss a range of solvent effects in hydrogenation reactions with respect to both the selectivity and activity. The effects will be examined in terms of mass transfer phenomena, the structure of the solvent and how the solvent may act as a co-catalyst.