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Introduction. Designing Heterogeneous Catalysts

Graham J. Hutchings[1] and C. Richard Catlow[1]

[1] Cardiff Catalysis Institute, School of Chemistry, Cardiff University, UK CF10 3AT

This feature issue concerns a collection of six articles all concerned with the topic of designing heterogeneous catalysts. Heterogeneous catalysis is the mainstay of the chemical industry as they are used for producing liquid fuels and chemical intermediates. As such they are essential for the manufacture of the greater majority of manufactured goods worldwide from pharmaceuticals to fertilisers. Indeed, it is considered that about half or the world's population is maintained by a single catalysed reaction, namely the fixation of nitrogen from the air to make ammonia and this involves an iron catalyst. In this way catalysis in general contributes about 20-25% of global GDP – it is therefore a topic of immense significance. Although we have many established catalysed processes that have been fully optimised, society is facing new challenges that require a more sustainable approach to how we utilise the planet's resources. This new drive in science requires new catalysts to be discovered and used if we are to meet the grand challenges we are facing. This feature issue deals with some of the approaches that are currently under investigation that we hope will set the stage for future technologies.

Charlie Fehl and Ben Davis describe the use of proteins as templates for complex synthetic metalloclusters: towards biologically programmed heterogeneous catalysis (DOI: 10.1098/rspa.2016.0078). They discuss the new dawn of de novo design of new metalloenzymes that will be a hybrid between homogeneous and heterogeneous catalysts and provide all the benefits of biocatalysts.

Alberto Roldan and Nora de Leeuw discuss the catalytic water dissociation by greigite Fe_3S_4 surfaces: density functional theory study (DOI: 10.1098/rspa.2016.0080). They discuss the use of greigite to activate CO_2 to form small molecules such as short chain acids. This could be particularly relevant to understanding the origin of life.

Richard Catlow and co-workers have investigated the reaction of formic acid with Raney™ copper (DOI: 10.1098/rspa.2016.0126). Copper catalysts are used in the industrial production of methanol for carbon monoxide and hydrogen, and surface formate is considered to be a crucial intermediate in this process. This paper explores this aspect of this important reaction.

Robert Raja and co-workers describe the influence of dopant substitution mechanism on catalytic properties within hierarchical architectures (DOI: 10.1098/rspa.2016.0095). They show how hierarchically porous AlPO-5 catalysts can be designed with isomorphously substituted transition metal ions and that the resulting active sites produced can influence the reactivity in the liquid-phase Beckmann rearrangement of cyclic ketones.

Chris Hardacre and Mike Bowker together with co-workers discuss hydrogen production by the photocatalytic reforming of cellulose and raw biomass using Ni, Pd, Pt and Au on titania (DOI: 10.1098/rspa.2016.0054). The quest for sustainable hydrogen production using sunlight and biomass is a current grand challenge in catalysis and this article describes some of the approaches that are possible.

Graham Hutchings and co-workers discuss the direct synthesis of hydrogen peroxide in water at ambient temperature (DOI: 10.1098/rspa.2016.0156). This reaction has a potential application in the disinfection of water but the challenge is controlling the selectivity of hydrogen utilisation as catalysts can decompose or hydrogenate hydrogen peroxide. This paper describes these challenges.

We hope that these papers in this special feature issue will create general interest in the topic of designing heterogeneous catalysts that will stimulate future research.