Centre for Sustainable & Circular Technologies

Centre for Sustainable and Circular Technologies; University of Bath

Project Title:	Stable Silica Based Strong Acids
Lead Supervisor and co-supervisors:	Professor Matthew Davidson (Lead Supervisor), Professor Janet L. Scott (Co-supervisor), Dr Pawel Plucinski (Co-supervisor), Dr Paul Murray (Industrial Supervisor)
Industrial Partner:	PhosphonicS Ltd

Project Summary

Background: There are a number of silica based acid catalysts available on the market. The acids have short term stability and can easily be used in a batch processes, but for continuous processes the functionality is not stable enough. Polymer based acids have better stability but poor wettability. There is a desire for a more stable silica based acid catalyst.

There are significant drivers, particularly in China, where significant quantities of bulk chemicals are manufactured, to move away from the large quantities of strong acids being used in industrial processes and to employ potentially cleaner processes. Using a solid supported acid catalyst rather than a liquid acid has a number of benefits including: waste reduction, recyclability of the acid catalyst, simplification of the product isolation; and reduction of the unit operations required (by 75% in some cases).

Proposition: Here we propose to develop flow processes for the efficient synthesis of a range of dipodal silanes,[1] that can be used to coat silicas, yielding stable materials.[2] Once the stability of the product is established, acid functionality will be introduced, either via the starting dipodal silane, or via post synthetic modification, and the product tested as an industrially relevant strong acid catalyst.

In more detail, this will entail, synthesising and characterising new dipodal silanes and developing processes in suitable flow reactors that allow close control of pressure, temperature, mixing and residence time. Close examination of reaction product distribution and kinetic data will be used to optimise the flow processes and thus to efficiently produce the range of dipodal silanes required. PhosphonicS are experts at the production of silica based materials and the dipodal silanes will be employed to coat known silicas and the stability will be examined. As enhanced stability is postulated to be a function of reduced mobility of the partially hydrolysed product, examination of equilibrium constants of hydrolysis will be used to compare materials and (re)design dipodal silanes. Finally, acid functionality will be introduced to the most stable materials and benchmarked

[1] B. A. Janeiro, B. C. Arkles, *United States patent US2007/0060765*, 15 March 2007

[2] B. Arkles, Y. Pan, G. L. Larson, M. Singh, *Chem. Eur. J.*, 2014, **20**, 9442 – 9450

against currently used liquid catalysts on industrially relevant starting materials, e.g. in alkylation or acylation reactions.

The PhD student will work both at the University of Bath and at PhosphonicS site in Compton as appropriate and will thus have the opportunity to develop industrial experience and networks during their PhD research.

Sustainability issues addressed

This project aims to produce an industrially relevant strong acid catalyst which will bring a number of sustainability benefits: waste reduction, recyclability of the acid catalyst, simplification of the product isolation; and significant reduction of the unit operations required.