Inorganic Materials & Catalysis

Research Project – Emiel Hensen - Ferdy Coumans

INORGANIC MATERIALS & CATALYSIS

Upgrading of bio-derived furanics *via* Diels-Alder Cycloaddition

Background

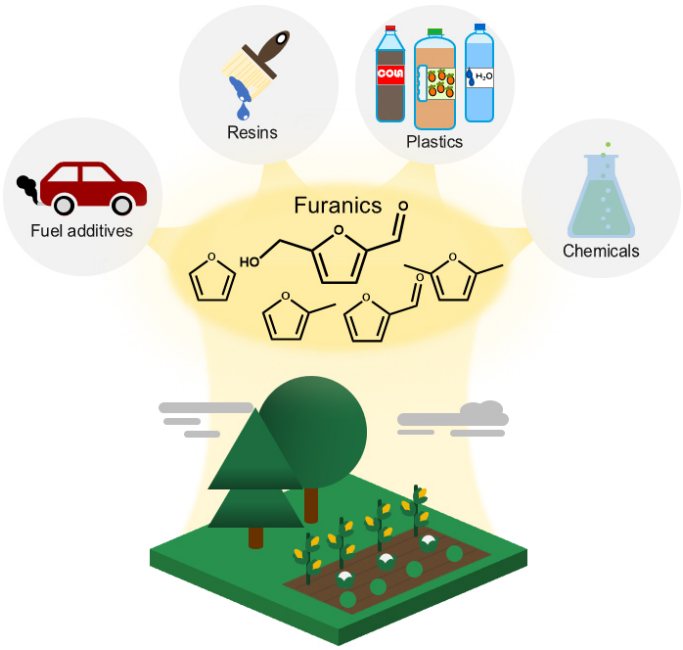

Figure 1. Bioderived furanic compounds as suitable building blocks for the chemical industry.

In recent years the replacement of chemicals from non-renewable origins with biobased compounds has been acknowledged as an effective solution for the environmental concerns. One such molecule that received significant attention is the sugar-derived *5*-hydroxymethylfurfural (*5*-HMF). This compound can be used to synthesize either petroleum-identical counterparts (drop-in) or novel replacement molecules that retain most of their natural functional groups. For example, the formation of para-xylene (*p*-xylene) from *2,5*-dimethylfuran (2,5-DMF) and ethylene is very appealing due to the intrinsic reaction mechanism of Diels-Alder Cycloadditions.[1] A high para-selectivity is desired to circumvent tedious purification steps as *p*-xylene is essential for the production of terephthalic acid and subsequent polyethylene terephthalate (PET). However, current processes are still hampered by low productivity, making them more expensive and even less environmentally friendly than fossil-based routes.[2] Thus, opening up possibilities to improve current and devise new catalytic methodologies in order to comply to the Green Chemistry standards.

Objectives

- Application of novel protection strategies for the valorisation of reactive furanic compounds
- Transforming high pressure batch reaction into a 3-phase flow process
- Exploratory studies to identify potential new pathways

Learning outcome

- Synthesis and characterization of heterogeneous catalysts
- High pressure catalytic testing using autoclaves and flow setup
- Incorporating organic synthetic procedures for heterogeneous reactions
- Characterization of reaction intermediates and catalysts using different techniques
  - NMR (liquid & solid), GC (-MS), HPLC, XPS, XRD, FTIR, Ar Physisorption
- Independent working and thinking

Further information

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[1] A. E. Settle, L. Berstis, N. A. Rorrer *et al*., Green Chem., *2017*, **19**, 3468-3492.
[2] Z. Lin, V. Nikolakis, M. Ierapetritou, Ind. Eng. Chem. Res., *2015*, **54**, 2366-2378.