SINCHEM 2017 doctoral research subject

Upgrading bio-platform molecules in the gas-phase: from levulinic acid to bio-chemicals

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PROJECT DETAILS:

Bio-based Building Blocks (B^4) obtained from lignocellulosic biomass are the starting reactants for the production of a variety of bio-chemicals and bio-fuels components. Upgrading of B^4 may be carried out either in the liquid or in the gas-phase, using properly designed catalysts. When carried out in the gas-phase, advantages include an easier separation of products, because of the absence of the solvent, an easier recovery and reuse of the catalyst, and the possibility to better integrate several successive steps in the aim of developing one-pot transformations. In this regard, the use of multifunctional catalysts is the key to perform complex multi-step reactions involving different type of active sites, such as acid/basic and redox sites.

The Project here outlined is aimed at studying the valorisation of levulinic acid (LA) into chemicals by means of gas-phase reactions. LA can be obtained from hexose monosaccharides, via intermediate formation of hydroxymethylfurfural; it can be transformed into chemicals such as γ-valerolactone and valeric acid, by means of liquid-phase processes involving successive steps of hydrogenation and dehydration.

The aim of this project is to explore the possibility of carrying out innovative processes for the transformation of LA in the gas-phase; examples of reactions which can be investigated include:

(a) oxidation of LA to produce maleic anhydride,

(b) (cascade) hydrodeoxygenation/dehydration of LA to produce pentanediols and methyltetrahydrofuran; the reaction will also be carried out using alcohols as H-transfer reagents.

(c) (cascade) hydrodeoxygenation/dehydration to produce aliphatic C4 and C5 hydrocarbons.

The PhD student will design and prepare catalysts for these reactions, using advanced preparation methodologies aimed at the synthesis of multifunctional, hierarchically-structured multicomponent systems. Catalysts will be characterised by means of different techniques, aimed at the identification of both structural and surface features, and will be tested for catalytic performance. Reactivity experiments will also be carried out in the liquid phase, in the aim of finding relationships between catalytic behaviors for reactions carried out under different conditions.