



## Wolfson Department of Chemical Engineering Seminar

Monday, November 25<sup>th</sup>, 2024 at 13:30

Room 4

### Identify a benchmark catalyst for deoxydehydration reaction of 1,2-propanediol to propylene

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Mid-PhD Seminar

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Nowadays, the chemical industry is mainly dependent on fossil resources to produce important building block molecules such as olefins. However, the gradual depletion and the ecological problems of fossil resources promotes the exploration of alternative sustainable resource, such as non-edible biomass. Among the non-edible biomass derived molecules, polyols are the most abundant and versatile substrates. These molecules typically carry primary or secondary hydroxyl groups with similar reactivities, which limits the selective transformation of polyols. Deoxydehydration (DODH) reaction has emerged as a new approach for generating synthetically useful olefins from polyols. Till now, rhenium-based catalysts have been recognized as the most promising catalysts for promoting DODH, attributed to their superior catalytic performance for different polyol molecules. However, the main challenge lies in the lack of a stable benchmark catalyst for DODH, which makes the comparison of catalysts or assessment of novel catalysts impossible.

Trioxo( $\eta^5$ -pentamethylcyclopentadienyl) rhenium ( $\text{Cp}^*\text{ReO}_3$ ) has received very limited attention despite being reported to be the first active catalyst for DODH in 1996. In this work, we identify  $\text{Cp}^*\text{ReO}_3$  as a potential stable benchmark homogeneous catalyst since it's well known that the  $\text{Cp}^*$  ligand can stabilize high oxidation state metals. Our study focuses on DODH of 1,2-propanediol, a substrate which can be readily produced from biomass waste derived glycerol. For the first time, we showed that  $\text{Cp}^*\text{ReO}_3$  is active for DODH of 1,2-propanediol to produce propylene with 100% selectivity. FTIR, MS were applied to analyze the gas phase while  $^1\text{H}$  NMR and UV-Vis were applied for liquid phase products analysis. The catalyst stability of  $\text{Cp}^*\text{ReO}_3$  during the course of DODH was rigorously investigated through the quantification of active rhenium species.

Refreshments will be served at 13:15.