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Mechanistic study of O_3-driven oxidation of alcohols: influence of oxygen carrier

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Aim

The aim of this project is to develop a mechanistic understanding of O_3-driven catalytic oxidation of alcohols, with a focus on how catalyst composition governs selectivity. The role of oxygen carrier components will be examined **experimentally** by systematically varying their composition and loading.

Justification

Global changes in energy production and consumption require a reconsideration of the chemical industry. In this context, aldehyde production, which is currently based on alkene transformation can be fundamentally rethought. To reduce fossil fuel consumption, the development of effic ient pathways for aldehyde production from renewable feedstocks has become essential.

Bioethanol is a promising renewable feedstock that can be used for the production of valuable chemicals, including acetaldehyde. Today, ethanol oxidation is already an industrial route for acetaldehyde production in regions with significant bioethanol availability. However, improvements in selectivity, heat management, and overall process efficiency are required to meet modern industrial standards.

Within the current trend toward electrification, conventional heat supply can be replaced by electrical energy. Gas phase **electrification** is often associated with plasma catalysis, which typically suffers from low selectivity. An alternative approach involves using plasma energy for preliminary oxygen activation, generating **ozone** that is subsequently fed into the catalytic reactor. Our recent results demonstrate that this strategy, combined with an appropriate catalyst, enables acetaldehyde **selectivity** and ethanol convevertion of **~ 90 % both at temperatures below 200 °C.**

This project will focus on studying the influence of oxygen carrier components with the aim of further improving selectivity and reducing the operating temperature.

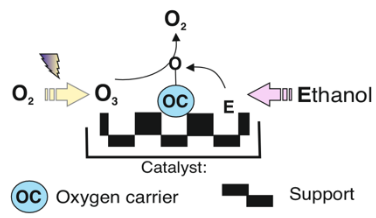

Figure 1. Reaction scheme

Figure 2. The setup for O_3-assisted oxidation studies

Program

The experimental plan includes:

1. Development of catalysts aimed at enhanced and selective ethanol oxidation.
2. Characterization of catalysts (STEM-EDX, XRD, chemo- and physisorption).
3. Evaluation of the catalytic properties in O_3-assisted ethanol oxidation.
4. Microkinetic modeling of ethanol oxidation over the best-performing samples.

The literature survey focuses on:

1. The importance of selective alcohol-to-aldehyde transformation for the pharmaceutical industry.
2. Alcohol-to-aldehyde pathways: dehydrogenation and oxidation.
3. Oxygen carriers: the most common materials (MnO_2, V_2O_5, CeO_2) and the nature of their properties.
4. The importance of and approaches to microkinetic modeling.

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