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SAPONITE-BASED CATALYSTS FOR THE CONVERSION OF ETHANOL TO 1,3-BUTADIENE

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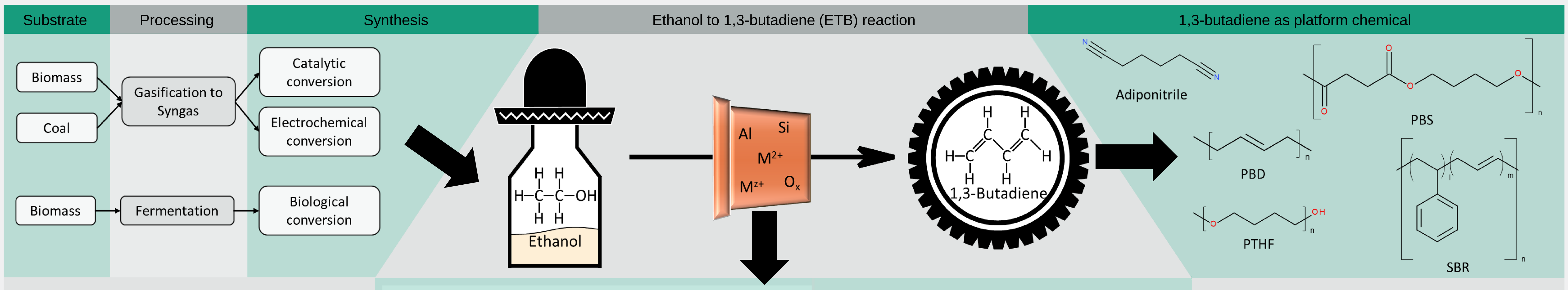
Introduction

1,3-butadiene (BD) is a platform chemical for the production of a broad range of polymers. The steam cracking of naphtha to ethylene is the main source for BD. Currently, shell gas replace naphtha as substrate for the ethylene production leading to a decreased BD production. Hence, a productive and sustainable process for the production of BD is required. The reaction of ethanol to BD (ETB) is a promising approach.
The ETB mechanism is complex and requires a catalyst containing balanced proportions of functional groups (see adjacent Table 1). Due to this issue a potential catalytic system for the ETB reaction is investigated.
Clay minerals, such as zeolites and saponites, are promising materials for the catalytic system. Saponites, layered aluminosilicates, are chosen as the catalytic system for the ETB reaction due to their high specific surface area, surface acidity and cation exchangeability. Furthermore, modification of saponites is possible using impregnation methods to generate the desired catalytic centres for the different steps of the ETB reaction.[1,2]

Reaction steps:
1) Oxidation of ethanol to acetaldehyde
2) Aldol addition/condensation to acetadol/crotonalaldehyde
3) Meerwein-Pondorf-Verley reaction
4) Dehydration
Requirements on the catalyst:
For 1) RedOx or basic centers
For 2) Lewis acid centers (accepting an electron pair) or basic centers
For 3) Lewis acid centers or basic centers
For 4) weak acidic (Brønsted) centers

Table 1 : Reaction steps and required catalytic centers for the ETB reaction.[3,4]



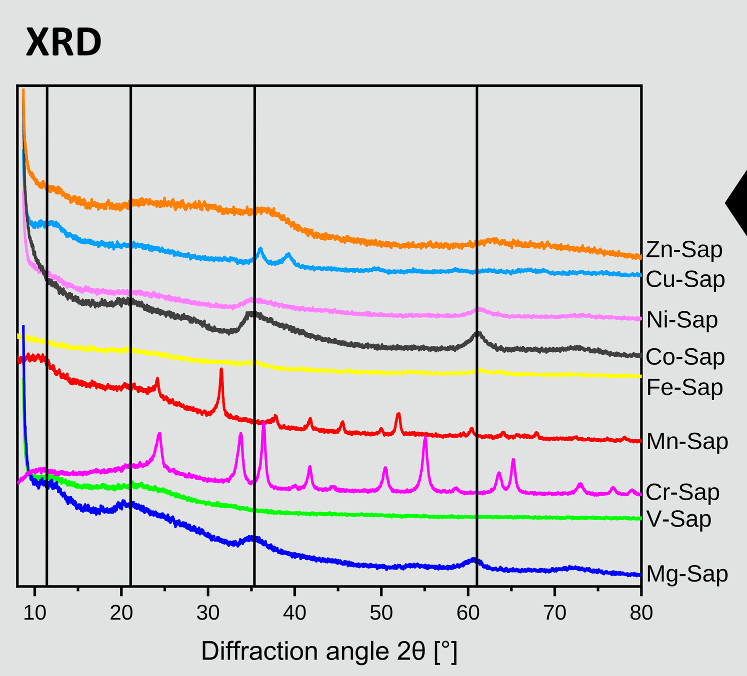


Fig. 2 : X-ray diffraction diffractograms of the synthesized saponite-based catalysts.

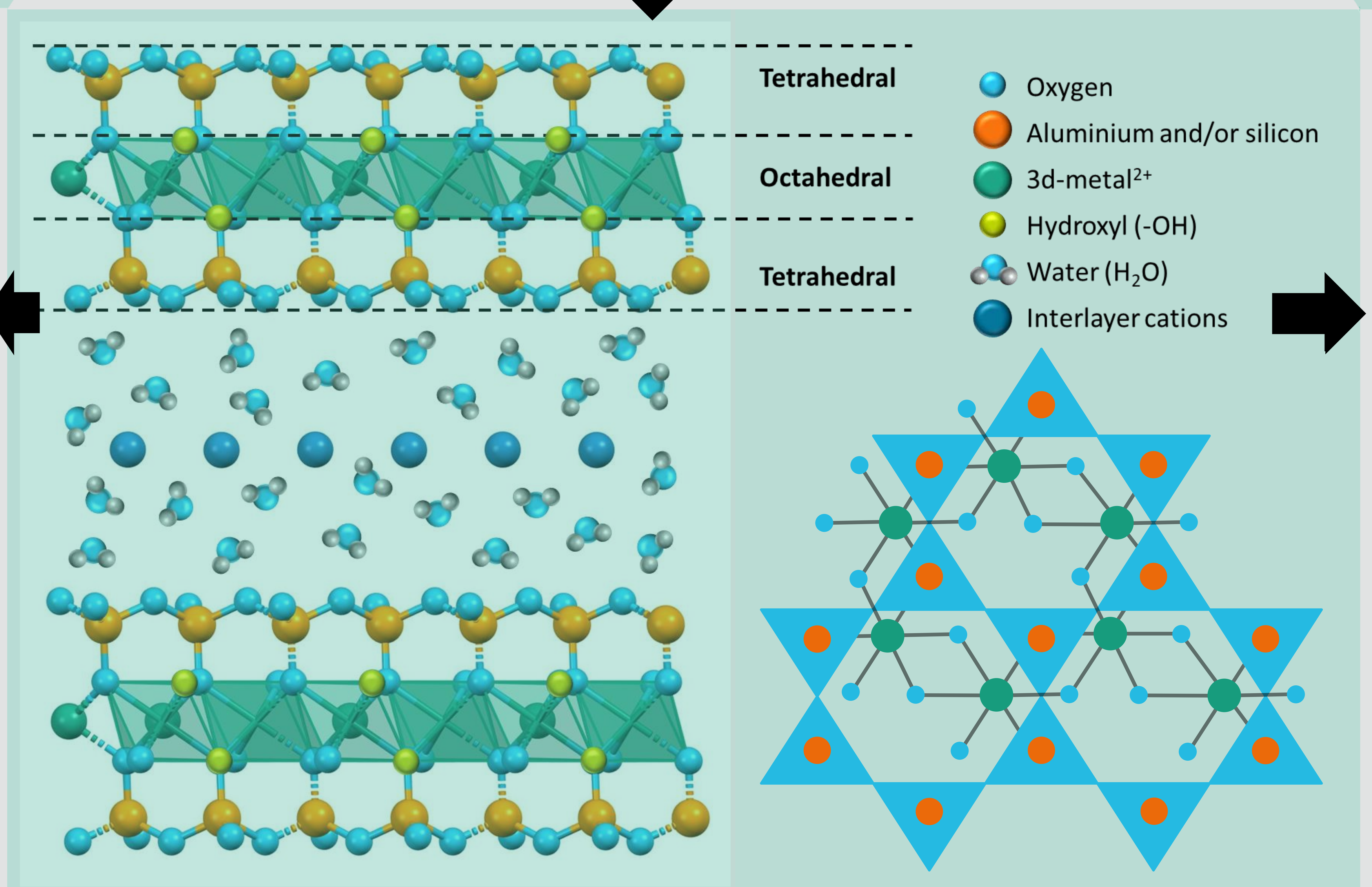


Fig. 1 : *Left:* Side view on a saponite crystal structur, two tetrahedral sheets containing Si^{4+} and/or Al^{3+} (orange) surrounding a central octahedral layer of divalent metals (green) and/or Al^{3+}; blue spheres represent oxygen atoms, hydrogen atoms are grey and yellow spheres show hydroxyl groups; interlayer cations (e.g. Na^+, Ca^{2+}) (blue) compensate negative charges in the layered structure and are highly hydrated. *Right:* Top view on the saponite crystal structure.[5]

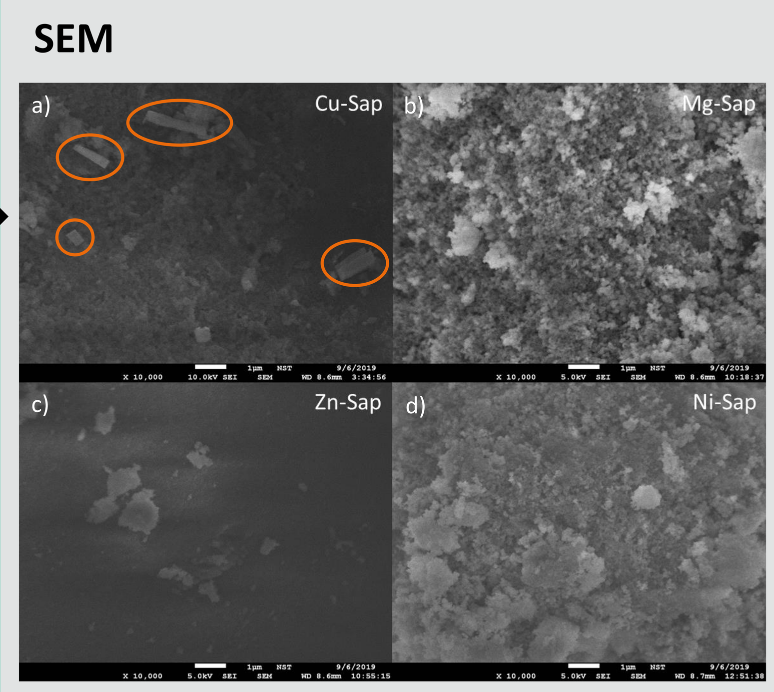


Fig. 3 : Scanning electron microscopy (SEM) images of saponite-based catalysts.

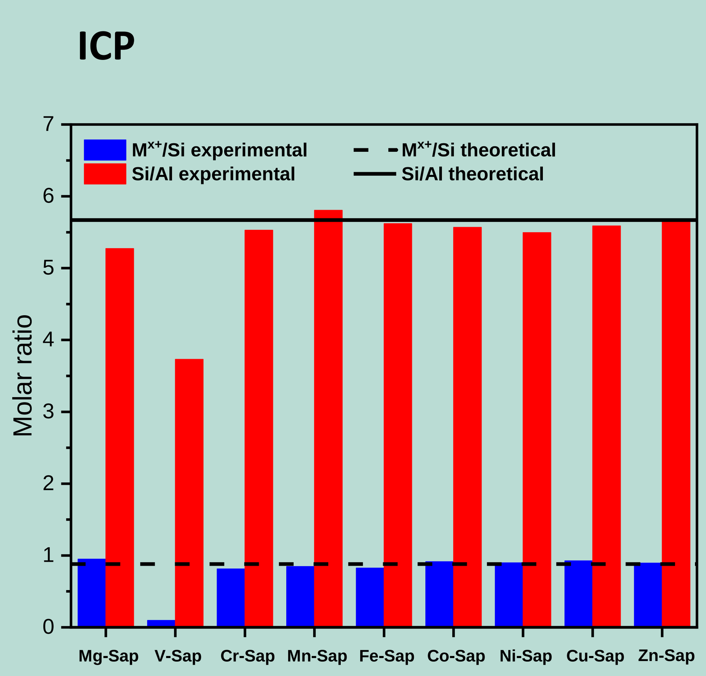


Fig. 4 : Results of inductively coupled plasma-optical emission spectrometry (ICP-OES).

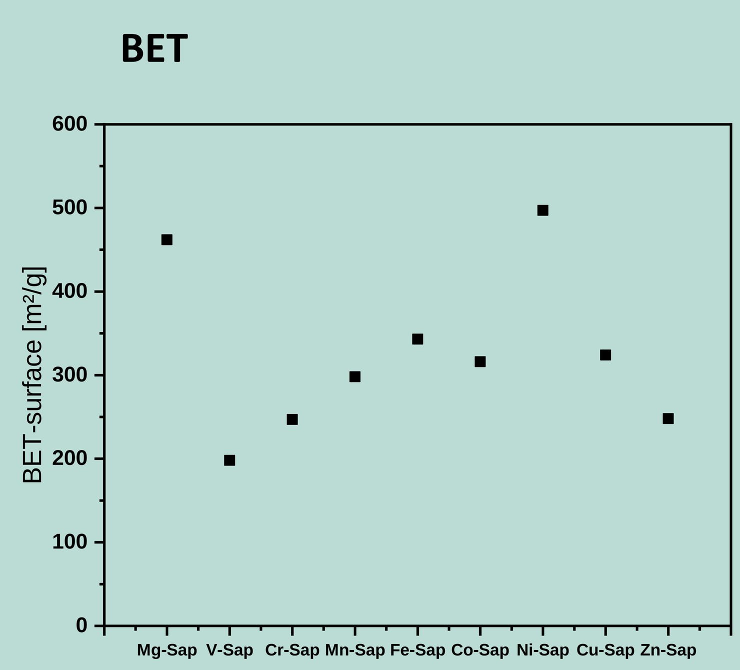


Fig. 5 : Nitrogen physisorption results of the saponite-based catalysts.

SUMMARY AND OUTLOOK

- Saponite-based materials containing different transition metals were successfully synthesized → catalysts are going to be tested in the ETB reaction
- Characterization of the materials using XRD, ICP, SEM and BET was conducted → further characterization for acid-base properties and thermal behaviour
- First structure-activity correlations were observed → determination of correlations on the catalytic effect
- Saponites show high potential as catalysts due to high adaptability → further modification and optimization after catalytic test

IN COOPERATION WITH

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