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ETRI 2023

BOOK OF ABSTRACTS



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Methodology: Initially, pseudobrookite (Fe_2TiO_5) was synthesized by a solvothermal method, reported by Melo et al. (ACS Appl. Nano Mater. 2020, 3, 9303–9317) with modifications, using $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and titanium isopropoxide in isopropanol. The formation of nanoparticles was achieved after calcination at 600 °C. In the following step, copper was incorporated into Fe_2TiO_5 structure by a solvothermal method using copper acetate as the precursor to produce materials Cu-loaded Fe_2TiO_5 , in proportions varying from 1 to 20% wt Cu.

CO_2 reduction was performed in an airtight quartz photoreactor under irradiation with a Xenon lamp. CO_2 (5 mL min⁻¹) was bubbled in a suspension containing 25,0 mg of the catalyst in 50 mL of 0,1 mol L⁻¹ NaHCO_3 for ~6h. The mixture catalyst + sodium bicarbonate solution was purged with argon (30 mL min⁻¹) for 30 min prior to the reaction. The gaseous products were analysed using an 8890 gas chromatograph (Agilent).

Preliminary results: Results under evaluation.

Preliminary conclusions: Work in progress.

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Abstract Title: Evaluation of catalysts derived from MgFe-pyroaurite structure impregnated with potassium in the hydrogenation of CO_2

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Abstract: In this study, MgFe catalysts derived from the structure of layered double hydroxides (LDHs), enhanced with potassium atoms (K), were investigated in the reverse reaction of the Reverse Water Gas-Shift

(RWGS) reaction. Based on the results obtained, it was observed that the addition of potassium led to a decrease in CH_4 production, increasing selectivity towards CO. Additionally, it was demonstrated that the material, when not calcined before the impregnation process with 5% (w.t.) of K, exhibited better catalytic performance than catalysts calcined at 500 and 800°C. Given the unprecedented nature of this research, the present study demonstrates, for the first time in the literature to the best of our knowledge, the most suitable method for preparing

catalysts derived from the MgFe-LDH structure impregnated with K, aiming at CO₂ hydrogenation reactions such as RWGS.

Keywords: CO₂ hydrogenation, CO, MgFe-based catalysts.

Introduction and Objectives: Anthropogenic emissions of CO₂ are recognized as an urgent problem due to CO₂ being one of the primary contributors to the Earth's rising average temperature, ocean acidification, and the extinction of certain animal and plant species.

Research into green hydrogen and CO₂ as feedstocks for the production of intermediates and molecules of industrial interest, such as CO, methanol, and olefins, is becoming increasingly important. These technologies offer a promising opportunity to reduce CO₂ emissions and promote a cleaner and more sustainable economy. Among the products, CO production is crucial for the synthesis of liquid hydrocarbons and other chemicals. However, achieving high selectivity in low-temperature CO production remains a challenge.

To overcome such challenges, this work proposes the use of the three-dimensional and multi-interface structure of LDH as a multifunctional catalyst. The LDH structure provides fundamental characteristics for enhancing the selectivity and stability of the catalyst in the RWGS (Reverse Water-Gas Shift) reaction, such as atomic dispersion and closer proximity of different inserted metals. An LDH of the MgFe type with a molar ratio (M²⁺:M³⁺) of 3:1 was selected as a potential catalyst for the RWGS reaction. The choice of magnesium is based on its basic properties, which have the ability to enhance CO₂ adsorption near active sites. On the other hand, the choice of iron is due to its nature as a non-noble, low-cost, and widely available metal. Furthermore, a key property of iron in this catalyst is its atomic-level dispersion within the LDH structure. According to the literature, the smaller the iron particle size, the higher the selectivity for CO.

Methodology: The synthesis of the MgFe precursor was conducted as described by Gonçalves et al. [1]. After synthesis, the resulting material was impregnated with 5% (by mass) of potassium (K), both in its as synthesized form and after calcination at 500°C and 800°C in a synthetic air atmosphere. Following impregnation, all catalysts were calcined at 500°C in a synthetic air atmosphere. The obtained catalysts were characterized by X-ray diffraction (XRD), nitrogen adsorption/desorption, and transmission electron microscopy (TEM).

The CO₂ hydrogenation reactions were performed in a Microactivity Efficient system from PID Eng&Tech, operated at atmospheric pressure, a gas hourly space velocity (GHSV) of 3600 mL gcat⁻¹ h⁻¹, an H₂:CO₂ ratio of 3, and a temperature of 370°C. Prior to the reaction process, the catalysts were reduced in a H₂ atmosphere (30 mL min⁻¹) at 500°C for 1 hour. The entire reaction line was maintained at 195°C to prevent condensation of reaction products. Conversion values (X%) and selectivity to products were calculated as established in the literature.

Preliminary results: Based on the XRD results, it is possible to observe that the LDH calcined at 800°C exhibits diffraction peaks corresponding to the MgFe₂O₄ and MgO phases, while the

other catalysts only show peaks of the MgO phase [2]. This observation highlights that, even when derived from the same precursor, the calcination temperature affects the type of phase present in the catalyst during the impregnation with K. The analysis of N₂ adsorption/desorption revealed that the MgFe800/K catalyst has a surface area of 44 m² g⁻¹, half of the value observed in the MgFe/K and MgFe500/K catalysts, which was 85 m² g⁻¹. This result can be attributed to a greater compaction of the structure due to the formation of the MgFe₂O₄ phase, as evidenced by the XRD results.

Elemental mapping images obtained through EDX provide clear evidence of the uniform distribution of the elements Mg, Fe, and K throughout the sample, even after the calcination and reduction processes. The results of catalytic activity clearly demonstrate that the addition of K is crucial for increasing the conversion of CO₂ and the selectivity for CO. Additionally, it was determined that the catalyst prepared with K impregnation (MgFe/K) in its as-prepared state is the most advantageous option for the RWGS reaction, as it has a lower cost and shorter preparation time.

Preliminary conclusions: The results obtained demonstrated that the calcination temperature of the precursor directly influences porosity and the formation of the MgFe₂O₄ phase. Additionally, it was shown that the LDH structure promotes the uniform dispersion of cations, and the addition of K is important for increasing selectivity towards CO, with no need for prior treatments on the LDH to carry out the impregnation with K.

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Abstract Title: Enhancing Carbonate Formation in Basalts of the Serra Geral Formation

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