

Catalytic behavior of niobia species on oxidation reactions: insights from experimental and theoretical models

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Abstract This paper describes the preparation and use of a new class of material based on synthetic Niobia as catalysts in oxidizing reactions of organic compounds in aqueous medium. The reaction chemicals were carried out in presence of hydrogen peroxide (H_2O_2). The material was characterized with X-ray diffraction, XPS, and UV–Vis measurements. The organic molecule methylene-blue was used in decomposition study as probe contaminant. The analysis using the ESI-MS technique showed complete oxidation observed through different intermediates. This suggests the use of Niobia species as efficient Fenton-like catalyst in degradation reactions. Theoretical quantum DFT calculations were carried out in order to understand the degradation mechanism.

Introduction

It has been reported that niobium is interesting and important for some catalytic reactions, and then the research and development of niobium compounds in catalytic applications have increased in recent years [1]. However, the use of pure niobium oxides as a catalyst for the oxidation of contaminants in aqueous medium is scarce in bibliography. It

has been reported a study with niobium oxides as a catalyst for hydroxylation, but combined with an inorganic cation at high temperature [2]. In general, research focuses on the study of the catalytic performance of Nb_2O_5 impregnated with metal oxides [3]. The particular properties of the niobium, such as, redox properties, photosensitivity, acidity, and catalytic behavior [4], constitute the motivation to understand and use niobium for catalytic purposes. Some important materials were been used as catalyst supports or promoters, but we are interesting in the utilization of Niobia. The natural abundance of niobium in the Earth crust is about 20 ppm in mass. Distributed by country, Brazil is the main niobium supplier, providing about 60% of the world production. Despite of the increasing interest on applications of niobium compounds in many technological fields, the niobium chemistry is not as deeply dominated for other more common industrial metals, as in heterogeneous catalysis [5]. Niobium-based materials are effective catalysts in numerous reactions, such as pollution control, selective oxidation, hydrogenation and dehydrogenation, dehydration and hydration, photochemistry, electrochemistry, and polymerization. A remarkable application of niobium-based compounds is on oxidation catalysis such as Fenton reaction. Fenton reaction involving hydrogen peroxide and ferrous catalyst is currently one of the most powerful oxidizing reactions available [6].

The main purpose of this paper was to prepare a new class of material based on a natural niobium oxide (niobia) to act as catalyst on the textile dye oxidation through a Fenton-like mechanism. In addition, some experiments have been carried out in order to study the effects of natural and synthetic Nb_2O_5 on the degradation of organic dye in the presence of hydrogen peroxide. The reaction mechanism of the heterogeneous dye/niobia/ H_2O_2 system has been studied on-line by ESI-MS and theoretical calculations.

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