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Effect of Humidity and Oxygen Vacancies in Photocatalytic Air Treatment

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Extended Abstract

Indoor air quality is critical for health as the residents in urban areas spend about 90% of their time indoors. Volatile organic compounds (VOCs), like ethanol and acetaldehyde, from food, cleaning products, and building materials, are major indoor air pollutants. They can cause respiratory issues, headaches, and dizziness if inhaled at sufficiently high concentrations. Moreover, Long-term exposure to ethanol may lead to liver damage, kidney issues, and increased risk of cancer. Thus, efficient mitigation of these compounds is crucial for maintaining a healthy indoor environment [1].

In recent years, photocatalysis has gained interest for environmental remediation [2]. Zinc oxide (ZnO) stands out as a popular photocatalyst due to its cost-effectiveness, non-toxicity, and strong removal capabilities [3]. However, challenges like its high bandgap, vulnerability to photocorrosion, and rapid recombination of electron-hole pairs limit its effectiveness [4]. Recent research indicates that modifying surface oxygen defects can enhance semiconductor catalysts' photocatalytic activity. These defects serve as charge traps and adsorption sites, facilitating efficient electron transfer to adsorbates and reducing electron-hole recombination [5].

An in-depth kinetic model was performed to examine the factors and mechanisms governing the photocatalytic degradation of gaseous ethanol, employing ZnO catalyst in an air purifier. The kinetic model that was developed from our previous model considering photocatalytic water treatment [6], concurrently monitors the concentrations of ethanol and its primary oxidation by-product, acetaldehyde, in both the gaseous phase and on the surface of the catalyst. It considers the reversible adsorption of these compounds to determine kinetic reaction parameters for various degradation pathways. The impact of oxygen vacancies on the catalyst was confirmed by comparing the catalytic performance of commercial ZnO before and after reduction pre-treatment (10% H_2/Ar gas at 500°C). Additionally, the effect of humidity was evaluated by analysing the distribution of water molecule concentrations in the gas phase and on the catalyst surface interface. Recognizing the significant role of adsorption in photocatalytic processes, the initial stages of all experiments (15 minutes in dark) were integrated into the model. Findings indicated a noticeable decrease in the adsorption removal of ethanol and acetaldehyde with increasing relative humidity from 5% to 75%. The estimated quantity of active sites, as determined by the model, demonstrates a significant increase after hydrogen reduction of ZnO. Furthermore, the model suggests that the reaction primarily occurs on the catalyst surface, with only 14% occurring in the gas phase. Finally, by using quantum yield calculations, the optimal humidity level for photocatalytic degradation was selected at 25%.

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