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Adsorption of SO_2 and NO_2 on ZrO_2 (1 1 0) Surface: Density Functional Theory and Molecular Dynamic Simulation Studies

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ABSTRACT

In order to save the environment, there is an urgent need for control measures due to the rapidly rising concentration of greenhouse gases in the atmosphere. Density functional theory (DFT) and molecular dynamic simulation investigations were used in this study to examine the adsorption characteristics of SO_2 and NO_2 on zirconia surface. Several global reactivity parameters where analyzed as part of the DFT calculations. Compared to NO_2 (ΔE = 6.424eV), the zirconia surface is substantially more sensitive to SO_2 (ΔE = 5.415eV) capture, according to the observed DFT data. The findings of the quenched molecular dynamic simulations also showed that SO_2 (E_{ads} = -66.23kcal/mol) is more likely to adsorb on zirconia surface than NO_2 (E_{ads} = -57.50kcal/mol), despite the fact that both molecules obey the physical adsorption mechanism. SO_2 and NO_2 respectively bond to the ZrO_2 (1 1 0) surface due to the two molecules' favorable orientation, which is parallel to the surface with angles pointing upward. Zirconium oxide can find use as an effective adsorbent for the removal of SO_2 and NO_2 gases from air environments because of these discoveries.

1. Introduction

The presence of SO_2 and NO_2 in the atmosphere has a significant impact on air pollution, including acid rain, photochemical smog, greenhouse effect, and ozone layer depletion [1]. When sulfur-containing fossil fuels are burned in factories, car engines, power plants, and homes, SO_2 gas is released into the atmosphere. Acid rain is created when the subsequent SO_2 gas mixes with atmospheric moisture [2]. However, high-temperature combustion processes, electrical discharge during thunderstorms, and microbiological activities in the soil all produce NO_2 gas [3]. The main antecedent of photochemical smog is the resultant NO_2 gas in the atmosphere [4].

To maintain a friendly environment, it becomes a global task to reduce the amount of greenhouse gases in the atmosphere [5]. Researchers spent a significant amount of effort and resources in developing effective methods to remove these dangerous gases from the environment [6]. Due to its low operating cost, effectiveness, simplicity of construction, and sensitivity towards gases, sensing gas molecules to capture the pollutant gases by adsorption is considered to be a method of choice. This is among the various methods developed to counteract the effect of greenhouse gases in the atmosphere [7]. Metal oxides have reportedly attracted a lot of attention among the various materials used to trap polluting gases from the atmosphere because of their wide range of applications [8].

Zirconia is a crystalline zirconium dioxide with mechanical characteristics resembling those of the metals to which it is analogous [9]. There are three different types of zirconia: mono-clinic, cubic, and tetragonal [10]. Numerous scientists have used experimental approaches, such as infrared spectroscopy and micro calorimetry techniques, to investigate the adsorption characteristics of gaseous contaminants on zirconia surfaces [11–13]. In hydrous zirconia gels, the origin of porosity was examined by Gimblett et al. [14].

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