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Adsorption of sulfuric acid on graphene with a high titanium coverage and on the [001] titanium surface

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Density functional theory and molecular dynamics were used to study the adsorption of sulfuric acid on two surfaces. One is graphene modified with titanium with high metal coverage (C_2Ti). The other is a [001] titanium surface. We considered cis and trans molecule conformers at 300 K, and atmospheric pressure. We found that the molecule (trans and cis) is dissociated and chemisorbed on the graphene-titanium layer, in several ways, forming a conductor surface. We also found that the molecule (cis and trans) is dissociated on the [001] titanium surface in only one, but a different way. In this case, all four oxygen atoms are chemisorbed, forming titanium oxide (TiO). The remaining sulfhydrylic acid is physisorbed, and it desorbs at 700 K.

1. Introduction

Sulfuric acid is a central substance in the chemical industry. It has a wide range of applications. Its principal uses include mineral processing, fertilizer manufacturing, oil refining, wastewater processing, chemical synthesis, electrolyte in lead-acid batteries, and various cleaning agents [1]. The interest in the properties of sulfuric acid originates in environmental problems such as acid rain and

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