



Adsorption of ammonia on ZrO_x -modified graphene nanoribbon: a first-principle investigation

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Abstract

Ammonia (NH_3) is a main environmental pollutant related to global warming, and reduction of its emission is the subject of multiple international agreements and regulations. Accordingly, the development of highly precise detectors to monitor its content in the environment is essential to track and limit its emission. This work examines the influence of modifying of armchair-graphene nanoribbon (AGNR) by zirconium (Zr) and its oxides on its adsorption for NH_3 gas. Density functional theory (DFT) computations are utilized to investigate the band structure, adsorption energy (E_a), adsorption length (D), charge transferred (ΔQ), and density of states (DOS) of pristine and modified structures with ZrO_x ($x = 0, 1$, or 2). ZrO_x is presented to AGNR nanostructure by two pathways: substitution of carbon atoms (doping) and introduction on top of the AGNR surface (decoration). The findings of the investigation illustrate great improvement of NH_3 adsorption on AGNR due to its modification. Although the adsorption energy is enhanced in general upon modification, AGNR structures where ZrO_x substitute carbon atoms exhibit greater adsorption energy as compared with the decoration scheme. The maximum energy of adsorption is for the AGNR structure doped with ZrO_2 , followed by that doped with Zr. The adsorption energy of NH_3 on the ZrO_2 -doped AGNR is -10.05 eV with an adsorption length of 2.4 Å and $-0.214e$ charge transferred. As compared to the pristine structure, the adsorption energy for NH_3 on AGNR doped with ZrO_2 increases 22.2 times. Therefore, AGNR nanostructure doped with ZrO_x can be considered for practical sensors for the applications of detection and control of ammonia emission.

Keywords Graphene nanoribbon · ZrO_x · Ammonia sensor · DFT

The abstract of the manuscript appears on the preprint of Research Square as it is submitted to a Springer journal. However, the manuscript (or part of it) was not published before neither it is under consideration in any other journal.

Highlights

1. AGNR is investigated for NH_3 gas adsorption using DFT calculation.
2. The effect of ZrO_x modification of AGNR structure through doping or decoration is examined.
3. The NH_3 adsorption capacity is tested by means of adsorption distance and energy, band structure, charge transferred, and DOS.
4. Excessive enhancement is observed towards NH_3 adsorption upon modification.
5. The adsorption energy of NH_3 on the ZrO_2 +AGNR is -10.05 eV, $D = 2.4$ Å and $\Delta Q = -0.214e$.
6. Adsorption energy towards ammonia for ZrO_2 +AGNR structure is 22.2 times more than that of the pristine.

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Introduction

Agricultural activities result 80–90% of the total global ammonia (NH_3) emission [1]. Its emission results mainly through volatilization of livestock manure as well as a synthetic mineral for nitrogen based fertilizers [2, 3]. NH_3 emissions alongside with other greenhouse gases that result mainly from agricultural activities have negative effects on air quality [4]. It is associated with two main environmental hazards: acidification and eutrophication [5]. When ammonia interacts with water, it increases the acidification of both soil and water [6]. Furthermore, the deposition of ammonia in soil and water can increase their nitrogen level that may increase the eutrophication of aquatic ecosystems [5]. Human exposure to ammonia concentrations of 25 ppm or higher may negatively influence the lung functions and respiratory track, and it may result injuries and risking burns for high exposure concentrations [7]. Accordingly, precise environmental monitoring of ammonia level and control of

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
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