Contents lists available at ScienceDirect

Kuwait Journal of Science

journal homepage: www.sciencedirect.com/journal/kuwait-journal-of-science

Full Length Article

Optimizing ethanol gas sensor with rGO layer addition on $LaFeO_3$–Pd doped material using density functional theory

Ahmad Aminudin [a], Rumaisya Az-zahra [a], Selly Feranie [a], Lilik Hasanah [a], Siti Kudnie Sahari [b], Endi Suhendi [a,*]

[a] Physics Study Program, Universitas Pendidikan Indonesia, Bandung, West Java, Indonesia
[b] Faculty of Engineering, Universiti Malaysia Sarawak, UNIMAS, Kota Samarahan, 94300, Sarawak, Malaysia

ARTICLE INFO

Keywords:
Gas sensors
$LaFeO_3$
Pd
rGO
Adsorption energy
Band gap

ABSTRACT

$LaFeO_3$ is widely applied in ethanol gas sensors due to material composition and the stability of its sensing parameters. However, $LaFeO_3$ is still limited in gas sensing properties, necessitating doping to enhance the performance of gas sensors like palladium (Pd). In this study, the optimization of the ethanol gas sensor was explored by adding reduced graphene oxide (rGO) to Pd–$LaFeO_3$, focusing on adsorption energy and band gap energy using density functional theory (DFT) with the generalized gradient approximation (GGA-PBEsol) simulation method. The results show that Pd–$LaFeO_3$ adsorption energy of −2.01 eV, which increases to −2.29 eV with the addition of rGO, indicates stronger ethanol adsorption. The band gap of Pd–$LaFeO_3$ was 2.34 eV before exposure to ethanol gas and decreased to 2.06 eV upon exposure. After incorporating rGO, the band gap further narrowed, from 0.11 eV before exposure to 0.05 eV after exposure. The narrowing of the energy band potentially enhances the sensor's response. Those results indicate that adding rGO to Pd–$LaFeO_3$ shows promising potential for ethanol gas sensor applications.

1. Introduction

The ease of evaporating ethanol has a negative impact on various fields, such as health and the environment. Exposure to ethanol vapours can cause significant air pollution, posing a risk to biodiversity and adversely affecting the function of neurobehavioral human (Ko et al., 2017). The harmful effects of ethanol gas necessitate the development of sensitive detection components, such as gas sensors, to monitor ethanol concentrations and mitigate its environmental impact. In the manufacture of sensors, metal oxide semiconductors are widely utilized in gas sensors due to their excellent sensitivity and compatibility, although selectivity and operating temperature are their main disadvantages (Uma and Shobana, 2023). Among these materials, $LaFeO_3$ is a widely used material in the manufacture of gas sensors.

$LaFeO_3$, a p-type semiconductor with an orthorhombic structure, is a highly attractive electroceramic material because of its excellent chemical stability at high temperatures, mixed ionic/electronic conductivity, and its strong sensing performance for gases such as acetone, formaldehyde, ethanol, SO_2, NO_2, CO, CH_4, CO_2, and O_2 (Jaouali et al., 2017). Its excellent gas sensitivity and high thermal stability make it a strong candidate for detecting various gases (Rong et al., 2018). While its stability and low phase formation temperature $LaFeO_3$ further enhance its potential as a sensing material (Ma et al., 2021). $LaFeO_3$ is widely used for detecting oxygen-containing gas molecules, as its oxygen deficiency significantly enhances its absorption capabilities and catalytic behaviour (Sharma et al., 2020). Its unique perovskite crystal structure and excellent gas sensing performance make it a subject of frequent study (Meng et al., 2024).

However, the gas-sensing performance of $LaFeO_3$ is limited by its low response and insufficient detection limit, which restricts its applicability for large-scale deployment in gas sensor technology (Zhang et al., 2022). To address these limitations, doping with other materials has been proposed as an effective solution. For instance, doping with metals like palladium (Pd) enhances its surface area and catalytic properties, resulting in exceptional reduction activities attributed to its oxygen storage capacity (Basahel et al., 2022). The Pd doping into graphene material results in strong chemisorption adsorption and enhanced gas sensing capabilities (Lu et al., 2023). Thus, in this study, Pd is added as a dopant in $LaFeO_3$ to enhance its gas-sensing properties.

Reduced graphene oxide (rGO) is recognised for unique properties

* Corresponding author.
E-mail address: endis@upi.edu (E. Suhendi).

https://doi.org/10.1016/j.kjs.2025.100430
Received 26 October 2024; Received in revised form 7 March 2025; Accepted 19 May 2025
Available online 21 May 2025