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Enhanced Ethanol Gas Sensor Performance through Adsorption Energy Analysis of Gd-Doped $LaFeO_3$ with rGO Coating: A Density Functional Theory Study

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ABSTRACT

LaFeO3 (LFO) is commonly used as a material for gas sensor applications. However, the LFO material in ethanol gas sensor applications can still improve sensitivity and selectivity parameters. Gadolinium (Gd) doping is widely used in gas sensor applications to increase the sensitivity of gas sensors. In addition, reduced graphene oxide (rGO) materials are commonly used in gas sensor applications to increase gas sensors' selectivity, sensitivity, and working temperature. This study analyzed the effect of Gd doping (LGFO) and the addition of an rGO single layer on LFO material (LGFO@rGO) on sensitivity and selectivity based on the adsorption energy of the system with ethanol gas molecules. Density Functional Theory studies were conducted to yield insight into the LGFO or LGFO@rGO – ethanol gas interactions and the sensitivity and selectivity improvement by changing adsorption energy. Based on the analysis, the presence of Gd doping and single-layer rGO could increase the adsorption energy. The addition of the rGO layer showed an escalation of the adsorption energy of about 9.45%, 2.49 eV in the LGFO to -2.75 eV LGFO@rGO. This improved adsorption capacity translates to a higher sensitivity for detecting lower concentrations of ethanol gas. This result shows the potential of LGFO and LGFO@rGO as ethanol gas sensor materials.

INTRODUCTION

Ethanol represents a class of volatile, colorless, and flammable alcohols that taste sweet when combined with water (Wati, et al., 2017). It finds extensive application across diverse industries. Notably, ethanol produces various beverage products within the pharmaceutical, perfumery, food industry, cosmetic sectors, breath analysis, and traffic safety (Baharum et al., 2020; Nga Phan et al., 2022). It is a flammable gas with an explosion range of 6-12% (Ning et al., 2023) and constitutes a significant risk factor contributing to numerous traffic accidents (Fergus, 2007; Nishitani, 2019; Abhilash et al., 2019). This compels the need to control and monitor ethanol gas concentrations in the environment effectively. While previous research has explored gas sensors for ethanol detection, limitations remain in achieving the desired sensitivity and selectivity, especially at low concentrations (Fergus, 2007). This highlights the need for further investigation into tailoring the structural and morphological properties of gas-sensing materials to enhance their performance (Sun et al., 2018; Wang et al., 2022).

While perovskite may garner significant attention in contemporary scientific research, it is not novel. This material was discovered in the Ural Mountains in 1839 by Russian mineralogist Lev Perovski (Zhang et al.,

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2023). It has a generic formula ABX_3, where A stands for monovalent cations, B for divalent metal cations, and X for halide ions. Perovskite materials continue to attract significant attention due to their unique properties, including high absorption coefficient, excellent light-harvesting capabilities, high charge carrier mobility, high melting and decomposition temperature, microstructural and morphological stability, good reliability, and thermal stability (Atta et al., 2016; Enhessari & Salehabadi, 2016; Zhang & Zhao, 2020; Zhang et al., 2023; Zhou et al., 2021). These properties make them ideal candidates for a wide range of applications, including gas sensors (Fergus, 2007), solar cells (Zhang et al., 2023), LEDs (Pacchioni, 2021), lasers (Zhang et al., 2021), and photodetectors (Zhang et al., 2021).

$LaFeO_3$ (LFO) is a metal oxide semiconductor, one of the perovskite materials. LFO has been studied in various applications, such as photocatalysts (Khen et al., 2021), solid oxide fuel cells (Zhou et al., 2021), and effect transistors (Wu et al., 2019). LFO is also popular and well-considered as one of the potential materials for gas sensor applications due to its properties, such as good selectivity, sensitivity, and high response (Cao et al., 2020; Suhendi et al., 2022). Previous research has shown that LFO had an excellent response to various gases, including ethanol gas (Cao et al., 2019; Suhendi et al., 2021). Gas sensors based on LFO work by the change of conductivity caused by interaction between adsorbed gas molecules on the surface of the sensor. Because of this, the incorporation of dopants into LFO and the deposition of coating material onto its surface are promising strategies for enhancing the gas-sensing performance of LFO-based gas sensors. Heretofore, a substantial body of research has demonstrated the potential of Gd doping to significantly enhance the performance, detection range, selectivity, and stability of gas sensors (Çolak & Karaköse, 2022; Haryadi et al., 2022; Li et al., 2023). Moreover, numerous studies have highlighted the immense potential of Gd as a dopant in gas sensor materials. Considering these findings, this study endeavors to explore the utilization of Gd-doped LaFeO3 (LGFO)-based gas sensors.

Several studies have indicated that graphene can augment adsorption because of its exceptionally high surface area. Graphene also exhibited significant alterations in electrical resistance upon adsorption. Graphene can serve as a support material for gas sensors. One such graphene-based material, reduced graphene oxide (rGO), offers both affordability and high sensitivity. Previous studies have demonstrated the enhancement of gas sensor performance through graphene (Li et al., 2022; Maity et al., 2017). rGO possesses excellent charge-carrier mobility, making it an attractive option for developing electronic sensors (Dua et al., 2010; Schedin et al., 2007). With advantages similar to those of graphene, rGO has gained considerable interest as a gas sensor material due to its lower fabrication costs.

Additionally, rGO can be easily modified or fine-tuned to achieve desired characteristics (Fellah, 2021; Guo et al., 2018; Sharma et al., 2020). Based on these findings, the present study investigates the impact of introducing an rGO coating onto LGFO (LGFO@rGO) to enhance the gas sensor performance. Specifically, we analyzed the change in the adsorption energies of LGFO and LGFO@rGO in the presence of ethanol gas. We evaluated the effect of rGO on LGFO, which resulted in increased adsorption energy owing to the presence of a single layer of rGO.

This study explores the adsorption energy alterations between LGFO and LGFO@rGO upon interaction with ethanol gas using Density Functional Theory (DFT) calculations. By comparing the adsorption energies of these materials, we sought to assess the influence of Gd doping and rGO coating on their gas-sensing properties, specifically for ethanol detection. The

findings of this investigation will contribute to the development of advanced gas sensor materials with improved performance and selectivity for the detection of ethanol gas.

METHODS

The first principle in this study based on density functional theory (DFT) is performed using Quantum ESPRESSO with the projector-augmented wave (PAW) pseudopotential. The generalized gradient approximation with Perdew-Burke-Ernzerhof (GGA-PBE) functional described the electronic exchange and correlation effects. The orthorhombic LaFeO3 (LFO) structure employed in this study possesses lattice parameters of a = 5.58 Å, b = 5.61 Å, and c = 7.90 Å. This structure accommodates 4 La atoms, 4 Fe atoms, and 12 O atoms within its unit cell.

This study implemented Gd doping by substituting 50% of the La atoms in LFO, resulting in the $La_{0.5}Gd_{0.5}FeO_3$ (LGFO) composition. The rGO structure was designed as a single layer of 19 carbon atoms (C) arranged in five honeycomb rings (hexagons). The carbon atoms' last available bonds were saturated with hydrogen atoms (H), and one oxygen atom (O) was inserted into the graphene structure to form the rGO structure, as shown in Figure 1.

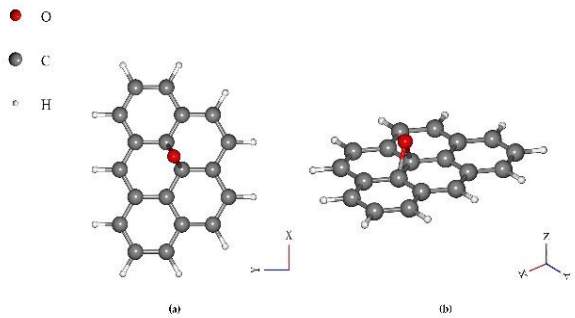

Figure 1 Schematic Illustrations of Single Layer rGO from (a) Top Side (b) Top-front Side

We employed a converged kinetic energy cutoff of 85 Rydberg, a converged k-point grid of 4x4x4, and an optimum distance between adsorbent and ethanol gas of 1 Å. These parameters were chosen based on convergence tests of the system's total energy. The optimum distance between adsorbent and ethanol gas of 1 Å was determined by performing calculations at different distances and comparing the corresponding adsorption energies.

The adsorption energy was calculated using equation (1), which has been widely used in previous studies (Sorescu, 2006; Timsorn & Wongchoosuk, 2020).

$$E_{adsorption} = E_{adsorban} + E_{adsorbate} - E_{system} \quad (1)$$

This equation accurately captures the interaction between the adsorbate and the adsorbent and provides a reliable measure of the adsorption strength. The research flowchart is shown in Figure 2.

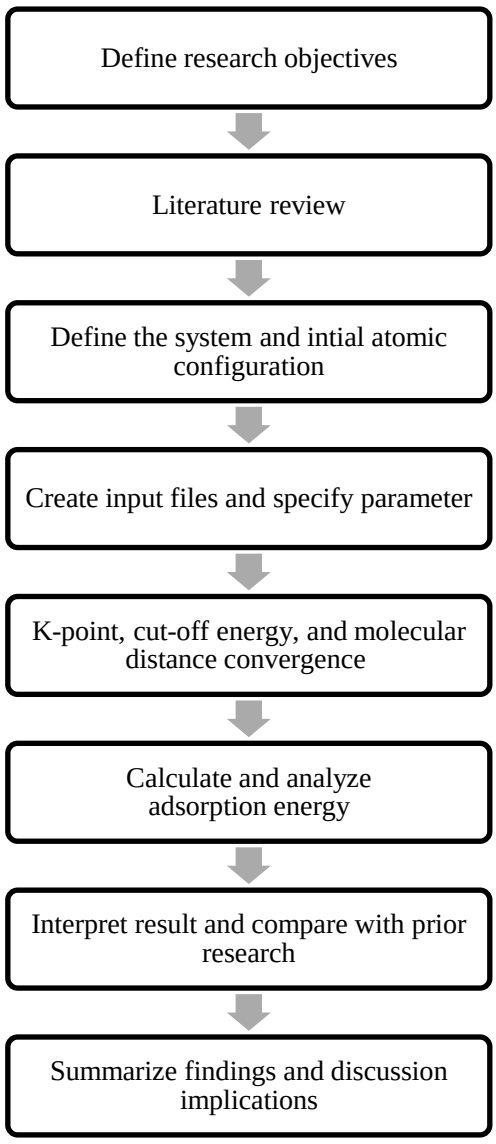

Figure 2 Research Flowchart

RESULTS AND DISCUSSION

The Ethanol Gas Molecule Adsorption at LGFO and LGFO@rGO Surface

The LaFeO3 crystal structure exhibits an orthorhombic arrangement with the space group Pbnm and contains 20 atoms within its unit cell. By substituting two La ions with Gd ions in the orthorhombic phase, LGFO is obtained. Figure 3 depicts the crystal structure of LGFO. The vc-relax calculations were performed to determine the adsorption energy of the ethanol gas molecule on LGFO. The calculations involved considering ethanol gas as the adsorbate, LGFO as the adsorbent, and the system consisting of LGFO interacting with ethanol.

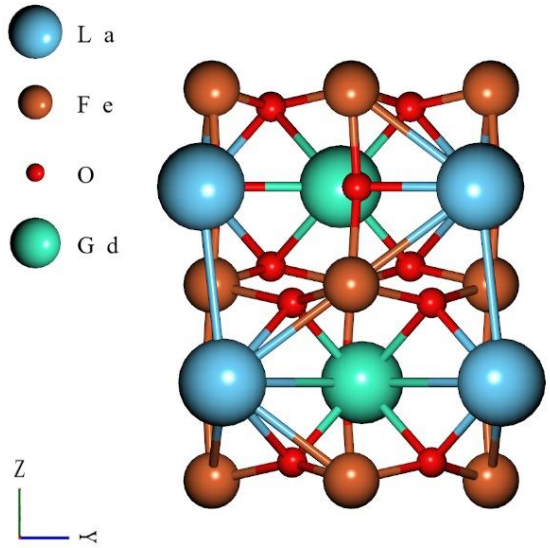

Figure 3. Schematic Illustration of LGFO

The vc-relax calculation for each adsorbate, adsorbent, and system provides the total energy, which is utilized in equation (1) to determine the adsorption energy of the ethanol gas molecule on LGFO. The research findings indicate an adsorption energy of -2.49 eV for the interaction between ethanol gas and LGFO. Moreover, when a single layer of rGO is added to LGFO as an adsorbate, as shown in Figure 4, the ethanol gas molecule adsorption at LGFO@rGO surface was found to be -2.75 eV.

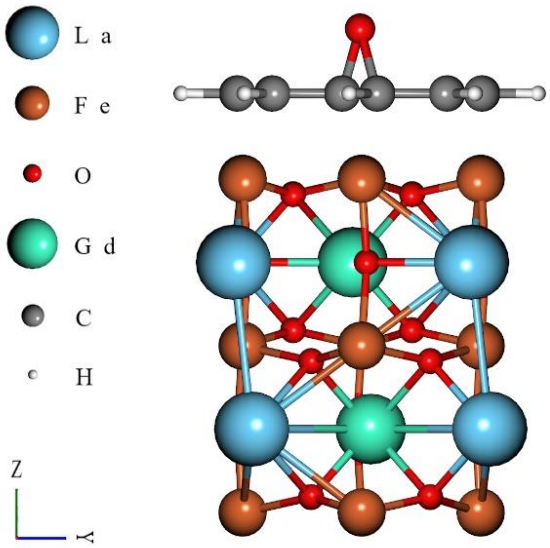

Figure 4. Schematic Illustration of LGFO@rGO

The negative adsorption energy values observed for both LGFO and LGFO@rGO indicate an exothermic reaction between the adsorbent and the adsorbate, resulting in a more energetically stable system (Cao et al., 2019; Chen et al., 2019; Li et al., 2019). Conversely, positive adsorption energy is typically unsuitable for gas sensor materials because it indicates an endothermic reaction. Positive adsorption energy values are unfavorable and imply that the material does not possess sensing properties for the gas molecules used as adsorbates (Al-Abbas et al., 2018; Joy et al., 2020; Kim et al., 2019; Wang et al., 2019). Additionally, the negative adsorption energy suggests a quick and spontaneous adsorption process on the surface of the adsorbent, which is favorable for gas sensors.

The Effects of rGO Coating on Adsorption Energy

The impact of rGO coating on the adsorption of ethanol gas on the LGFO surface is moderately enhanced. This enhancement is primarily due to the increased surface reactivity of the rGO, leading to enhanced adsorption energy. The improved adsorption enriched the capability of the ethanol gas sensor based on LGFO, enabling the detection of low concentrations of ethanol gas. The rGO coating introduces

additional active sites for binding ethanol gas molecules, resulting in enhanced adsorption energy. In this study, the adsorption energy was observed to augment 9.45% from -2.49 eV to -2.75 eV after rGO coating. The adsorption energies of the rGO-coated LGFO are more negative than those of the uncoated LGFO, indicating that the rGO coating on LGFO provides more stable configurations than the uncoated material.

The more negative adsorption energy post-rGO coating reveals a firmer connection between ethanol gas and LGFO@rGO than on LGFO. This attests that the ethanol gas molecules showcase greater adhesion affinity and are more apt to adhere to the LGFO@rGO surface. The more formidable correlation augmented the sensitivity of the gas sensor, permitting the detection of low concentrations of ethanol gas. The more negative the adsorption energy illustrates, the more robust the adsorption (Zhou et al., 2016).

The selectivity of a gas sensor can be assessed by comparing the adsorption energies of the different gases. Table 1 compares previous research results for various adsorbates and adsorbents for gas sensors. LFO and LFNO exhibited adsorption energies of -2.27 eV and -2.37 eV, respectively. Comparing these values with the present study on LGFO and LGFO@rGO, it is evident that the gas sensor based on LFO is more suitable for detecting ethanol gas than H_2.

In another study, the adsorption energy of ethanol gas on Ag metal decorated SnO_2 was found to be -1.82 eV. This comparison demonstrates that the ethanol gas sensor based on LGFO and LGFO@rGO is slightly more sensitive than the one based on Ag metal decorated SnO_2. This study's more negative adsorption energy suggests that LGFO and LGFO@rGO possess a higher affinity for ethanol gas. This selectivity can be advantageous when designing gas sensors for specific applications that require the detection of ethanol gas (Kou et al., 2014). A more negative adsorption energy signifies that the desorption process, involving releasing ethanol gas molecules from the sensor surface, is thermodynamically favorable. This reversibility is crucial for gas sensors as it allows them to be reusable and responsive to changes in ethanol gas concentration.

However, this research solely focuses on studying the potential of LGFO and LGFO@rGO in adsorption energy, owing to computational resource constraints for performing extensive DFT calculations. Therefore, further in-depth studies are required to investigate their potential for ethanol gas sensor applications, considering factors such as electronic properties. Modifying the rGO structure by introducing doping, as demonstrated in numerous research studies, could potentially enhance the overall performance of this gas sensor. Experimental research can also be conducted to compare the theoretical findings obtained through DFT calculations with practical results.

Consequently, this research highlights the promising potential of LGFO and LGFO@rGO for ethanol gas sensor applications.

Table 1. The Adsorption Energy of Various Materials for Various Gas Molecules

No.	Material	Gas	$E_{adsorptoin}$ (eV)	References
1	$LaFeO_3$	H_2	-2.27	(Zhou et al., 2021)
2	$LaFe_{0.75}Nb_{0.25}O_3$ (LFNO)	H_2	-2.37	(Zhou et al., 2021)
3	$LaFeO_3$	NO	-1.38	(Kizaki & Kusakabe, 2012)
4	Ag metal decorated SnO_2	C_2H_6O	-1.82	(Li et al., 2019)
5	ZnO	NO_2	-2.02	(Gao et al., 2021)
6	ZnO@rGO	NO_2	-2.46	(Gao et al., 2021)
7	LGFO	C_2H_6O	-2.49	this research
8	LGFO@rGO	C_2H_6O	-2.75	this research

With adsorption energies of -2.49 eV and -2.75 eV for LGFO and LGFO@rGO, respectively, these materials are generally considered favorable due to their negative adsorption energy. Furthermore, the LGFO@rGO composite exhibits slightly better sensing performance. The gas sensor's performance can be enhanced by incorporating rGO, which possesses a large surface area and more active sites. The findings of this study suggest that LGFO@rGO exhibits superior sensitivity and selectivity when detecting ethanol molecules in gas form, thus surpassing the performance of LFO or LGFO sensors. These results have significant implications for the practical deployment of ethanol gas sensors. The enhanced sensitivity and selectivity of the LGFO@rGO sensor design offer the potential for more accurate and reliable detection of ethanol across various applications. Additionally, the high sensitivity and selectivity of LGFO@rGO to ethanol gas molecule adsorption make it an attractive candidate for superior gas sensing applications.

CONCLUSION AND SUGGESTION

DFT Calculation studied the adsorption energy of LGFO and LGFO@rGO. The adsorption energies of ethanol on LGFO and LGFO@rGO are -2.49 eV and -2.75 eV, respectively. The results demonstrate that rGO coating on LGFO effectively enhances the adsorption energy of ethanol by 9.45%. This improved adsorption capacity translates to a higher sensitivity for detecting lower concentrations of ethanol gas. Therefore, LGFO@rGO holds promising potential as a material for susceptible ethanol gas sensors.

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AUTHOR CONTRIBUTIONS

MI contributed to software, formal analysis, investigation, data curation, writing original draft, and visualization. AS contributed to methodology and resources. W contributed to conceptualization and validation. TSM contributed to the formal analysis and writing the original draft. ES contributed to conceptualization, validation, methodology, writing, review, and editing. AA contributed to methodology, validation, resources, supervision, project administration, and funding acquisition.

REFERENCES

Al- Abbas, S. S. A., Muhsin, M. K., & Jappor, H. R. (2018). Tunable optical and electronic properties of gallium telluride monolayer for photovoltaic absorbers and ultraviolet detectors. *Chemical Physics Letters*, *713*(September), 46–51. https://doi.org/10.1016/j.cplett.2018.10.020

Atta, N. F., Galal, A., & El-Ads, E. H. (2016). Perovskite Nanomaterials – Synthesis, Characterization, and Applications. *Perovskite Materials - Synthesis, Characterisation, Properties, and Applications*. https://doi.org/10.5772/61280

Baharum, N. B., Daud Awang, M., Arshad, S., & Abd Gani, S. S. (2020). A Study of Literatures: Status of Alcohol in Cosmetics Products from Shariah Views in Malaysia. *KnE Social Sciences*, *2020*, 379–393. https://doi.org/10.18502/kss.v4i9.7338

Cao, E., Feng, Y., Guo, Z., Wang, H., Song, G., Zhang, Y., Hao, W., Sun, L., & Nie, Z. (2020). Ethanol sensing characteristics of (La,Ba)(Fe,Ti)O3 nanoparticles with impurity phases of BaTiO3 and BaCO3. *Journal of Sol-Gel Science and Technology*, *96*(2), 431–440. https://doi.org/10.1007/s10971-

020-05369-x

Cao, E., Wu, A., Wang, H., Zhang, Y., Hao, W., & Sun, L. (2019). Enhanced Ethanol Sensing Performance of Au and Cl Comodified LaFeO3 Nanoparticles. *ACS Applied Nano Materials*, *2*(3), 1541–1551. https://doi.org/10.1021/acsanm.9b00024

Chen, M., Wang, H., Hu, J., Zhang, Y., Li, K., Zhang, D., Zhou, S., Zhang, J., Zhu, Z., & Liu, Q. (2019). Near-Room-Temperature Ethanol Gas Sensor Based on Mesoporous Ag/Zn–LaFeO3 Nanocomposite. *Advanced Materials Interfaces*, *6*(1). https://doi.org/10.1002/admi.201801453

Çolak, H., & Karaköse, E. (2022). Gadolinium(III)-doped ZnO nanorods and gas sensing properties. *Materials Science in Semiconductor Processing*, *139*, 106329. https://doi.org/10.1016/j.mssp.2021.106329

Dua, V., Surwade, S. P., Ammu, S., Agnihotra, S. R., Jain, S., Roberts, K. E., Park, S., Ruoff, R. S., & Manohar, S. K. (2010). All-Organic Vapor Sensor Using Inkjet-Printed Reduced Graphene Oxide. *Angewandte Chemie*, *122*(12), 2200–2203. https://doi.org/10.1002/ange.200905089

Enhessari, M., & Salehabadi, A. (2016). Perovskites-Based Nanomaterials for Chemical Sensors. *Progresses in Chemical Sensor*, *August*. https://doi.org/10.5772/62559

Fellah, M. F. (2021). The reduced graphene oxide/WO3: Sensing properties for NO2 gas detection at room temperature. *Diamond and Related Materials*, *119*(2), 108593. https://doi.org/10.1016/j.diamond.2021.108593

Fergus, J. W. (2007). Perovskite oxides for semiconductor-based gas sensors. In *Sensors and Actuators, B: Chemical* (Vol. 123, Issue 2, pp. 1169–1179). https://doi.org/10.1016/j.snb.2006.10.051

Gao, H., Ma, Y., & Wang, Q. (2021). Gas sensor based on rGO/ZnO aerogel for efficient detection of NO2 at room temperature. *Journal of Materials Science ; Materials in Electronics*, *3*(1), 10058– 10069.

Guo, L., Hao, Y. W., Li, P. L., Song, J. F., Yang, R. Z., Fu, X. Y., Xie, S. Y., Zhao, J., & Zhang, Y. L. (2018). Improved NO2 Gas Sensing Properties of Graphene Oxide Reduced by Two-beam-laser Interference. *Scientific Reports*, *8*(1), 1–7. https://doi.org/10.1038/s41598-018-23091-1

Haryadi, H., Syarif, D. G., & Suhendi, E. (2022). The Effect of Couple Doping Gd and Co on The Physical Characteristics of LaFeO3 Thick Film for Acetone Gas Sensor Application. *Jurnal Penelitian Fisika Dan Aplikasinya (JPFA)*, *12*(2), 115–126. https://doi.org/10.26740/jpfa.v12n2.p115-126

Joy, R., Han, Z., Xu, K., Pan, X., Liao, N., & Zhou, H. (2020). DFT investigation of gas sensing characteristics of Au-doped vanadium dioxide. *Physics Letters, Section A: General, Atomic and Solid State Physics*, *384*(32), 2–6. https://doi.org/10.1016/j.physleta.2020.126823

Khen, L. Y., Mohtar, S. S., Aziz, F., Wan Salleh, W. N., Yusof, N., Jaafar, J., & Ismail, A. F. (2021). Floatable photocatalyst LaFeO3/modified expanded perlite composite for photocatalytic ammonia degradation. *Journal of Water Process Engineering*, *44*, 102401. https://doi.org/https://doi.org/10.1016/j.jwpe.2021.102401

Kim, Y., Choi, Y. S., Park, S. Y., Kim, T., Hong, S. P., Lee, T. H., Moon, C. W.,

Kou, L., Yang, T., Luo, Yaguang., Liu, X., Huang, L., & C. Eron. (2014). Pre-

harvest calcium application increases biomass and delays senescence of broccoli microgreens. *Postharvest Biology and Technology*, 87(1), 70–78.

Lee, J. H., Lee, D., Hong, B. H., & Jang, H. W. (2019). Au decoration of a graphene microchannel for self-activated chemoresistive flexible gas sensors with substantially enhanced response to hydrogen. *Nanoscale*, *11*(6), 2966–2973. https://doi.org/10.1039/c8nr09076a

Kizaki, H., & Kusakabe, K., (2012). DFT-GGA study of NO adsorption on the LaO (001) surface of LaFeO3. *Surface Science*, *606*(3–4), 337–43.

Wati, L., Goel. A., & Raj. K. (2017). Ethanol Production From Different Substrates: Effects On Environmental Factors And Potential Applications. In *Engineering Interventions in Foods and Plants* (pp. 211–246). Apple Academic Press.

Li, M., Zhu, H., Wei, G., He, A., & Liu, Y. (2019). *DFT calculation and analysis of the gas sensing mechanism of methoxy propanol on Ag decorated*. 35862–35871. https://doi.org/10.1039/c9ra02958c

Li, Y., Chen, K., Liu, Y., Ma, J., Liao, Y., Yang, H., Cheng, J., Yue, Q., Yuan, K., Ren, Y., Zou, Y., & Deng, Y. (2023). Gadolinium-doped mesoporous tungsten oxides: Rational synthesis, gas sensing performance, and mechanism investigation. *Nano Research*, *16*(5), 7527–7536. https://doi.org/10.1007/s12274-022-5274-6

Li, Y., Xu, Y., & Li, X. (2022). The sensing mechanism of HCHO gas sensor based on transition metal doped graphene: Insights from DFT study. *Sensors and Actuators A: Physical*, *338*, 113460. https://doi.org/https://doi.org/10.1016/j.sna.2022.113460

Maity, I., Ghosh, K., Rahaman, H., & Bhattacharyya, P. (2017). Selectivity Tuning of Graphene Oxide Based Reliable Gas Sensor Devices by Tailoring the Oxygen Functional Groups: A DFT Study Based Approach. *IEEE Transactions on Device and Materials Reliability*, *17*(4), 738–745. https://doi.org/10.1109/TDMR.2017.2766291

Nga Phan, T. T., My Dinh, T. T., Duc Nguyen, M., Dan Li, Nhan Phan, C., Kien Pham, T., Tu Nguyen, C., & Huyen Pham, T. (2022). Hierarchically structured LaFeO3 with hollow core and porous shell as efficient sensing material for ethanol detection. *Sensors and Actuators B: Chemical*, *354*, 131195. https://doi.org/https://doi.org/10.1016/j.snb.2021.131195

Ning, X., Zhang, Z., Zheng, K., Wang, X., & Wang, J. (2023). Experimental and Numerical Studies on the Explosion Characteristics of Ethanol–Air Mixtures under Aviation Conditions. *Fire*, *6*(9). https://doi.org/10.3390/fire6090349

Nishitani, Y. (2019). Alcohol and traffic accidents in Japan. *IATSS Research*, *43*(2), 79–83. https://doi.org/https://doi.org/10.1016/j.iatssr.2019.06.002

Pacchioni, G. (2021). Highly efficient perovskite LEDs. *Nature Reviews Materials*, *6*(2), 108. https://doi.org/10.1038/s41578-021-00280-5

Abhilash, K. P.P., Lath, D., Kowshik, J., Jose, A., & Chandy, G. M. (2019). Blood alcohol levels in road traffic accidents: Factors associated and the relationship between history of alcohol consumption and blood alcohol level detection. *International Journal of Critical Illness and Injury Science*, *9*(3), 132–137. https://doi.org/10.4103/IJCIIS.IJCIIS_45_19

Schedin, F., Geim, A. K., Morozov, S. V., Hill, E. W., Blake, P., Katsnelson, M. I., & Novoselov, K. S. (2007). Detection of individual gas molecules adsorbed on graphene. *Nature Materials*, *6*(9), 652–

655. https://doi.org/10.1038/nmat1967

Sharma, N., Kushwaha, H. S., Sharma, S. K., & Sachdev, K. (2020). Fabrication of LaFeO3 and rGO-LaFeO3 microspheres based gas sensors for detection of NO2 and CO. *RSC Advances*, *10*(3), 1297–1308. https://doi.org/10.1039/C9RA09460A

Suhendi, E., Amanda, Z. L., Ulhakim, M. T., Setiawan, A., & Syarif, D. G. (2021). The enhancement of ethanol gas sensors response based on calcium and zinc co-doped LaFeO3/Fe2O3 thick film ceramics utilizing yarosite minerals extraction as Fe2O3 precursor. *Journal of Metals, Materials and Minerals*, *31*(2), 71–77. https://doi.org/10.14456/jmmm.2021.21

Suhendi, E., Putri, A. E., Ulhakim, M. T., Setiawan, A., & Syarif, D. G. (2022). Investigation of ZnO doping on LaFeO3/Fe2O3 prepared from yarosite mineral extraction for ethanol gas sensor applications. *AIMS Materials Science*, *9*(1), 105–118. https://doi.org/10.3934/MATERSCI.2022007

Sun, Z., Zhang, Y., Liu, W., Wang, Y., & Ren, S. (2018). *Innovative Thought and Methodology of Planck Constant Experiment Based on Photoelectric Effect Theorem*. *221*(Ceed), 667–670.

Wang, H., Luo, W., Tian, Z., & Ouyang, C. (2019). First principles study of alkali and alkaline earth metal ions adsorption and diffusion on penta-graphene. *Solid State Ionics*, *342*(July), 115062. https://doi.org/10.1016/j.ssi.2019.115062

Wang, Y., Li, H., Huang, D., Wang, X., Cai, L., Chen, Y., Wang, W., Song, Y., Han, G., & Zhen, B. (2022). A high-performance ethanol gas sensor based on Ce-doped SnO2 nanomaterials prepared by the Pechini method. *Materials Science in Semiconductor Processing*, *137*, 106188. https://doi.org/https://doi.org/10.1016/j.mssp.2021.106188

Wu, T., Pisula, W., Rashid, M. Y. A., & Gao, P. (2019). Application of Perovskite-Structured Materials in Field-Effect Transistors. *Advanced Electronic Materials*, *5*(12), 1900444. https://doi.org/https://doi.org/10.1002/aelm.201900444

Zhang, H. C., & Zhao, X. . (2020). The role of oxygen vacancies of ABO3 perovskite oxides in the oxygen reduction reaction. *Energy & Enviromental Science*. https://doi.org/10.1039/D0EE00092B

Zhang, L., Mei, L., Wang, K., Lv, Y., Zhang, S., Lian, Y., Liu, X., Ma, Z., Xiao, G., Liu, Q., Zhai, S., Zhang, S., Liu, G., Yuan, L., Guo, B., Chen, Z., Wei, K., Liu, A., Yue, S., … Ding, L. (2023). Advances in the Application of Perovskite Materials. *Nano-Micro Letters*, *15*(1), 177. https://doi.org/10.1007/s40820-023-01140-3

Zhang, Q., Shang, Q., Su, R., Do, T. T. H., & Xiong, Q. (2021). Halide Perovskite Semiconductor Lasers: Materials, Cavity Design, and Low Threshold. *Nano Letters*, *21*(5), 1903–1914. https://doi.org/10.1021/acs.nanolett.0c03593

Zhang, Y., Ma, Y., Wang, Y., Zhang, X., Zuo, C., Shen, L., & Ding, L. (2021). Lead-Free Perovskite Photodetectors: Progress, Challenges, and Opportunities. *Advanced Materials*, *33*(26), 2006691. https://doi.org/https://doi.org/10.1002/adma.202006691

Zhou, Y., Lü, Z., Li, J., Xu, S., Xu, D., & Wei, B. (2021). The electronic properties and structural stability of LaFeO3 oxide by niobium doping: A density functional theory study. *International Journal of Hydrogen Energy*, *46*(13), 9193–9198. https://doi.org/10.1016/j.ijhydene.2020.12.202

Zhou, Y., Lü, Z., Wei, B., Xu, S., Xu, D., &

Yang, Z. (2016). The comparative theoretical study of the LaBO3 (001) (B = Mn, Fe, Co, and Ni) surface properties and oxygen adsorption mechanisms. *Ionics*, *22*(7), 1153–1158. https://doi.org/10.1007/s11581-016-1638-9