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6th International Conference on

Micro/Nanoelectronics Devices, Circuits and Systems

National Institute of Technology Silchar

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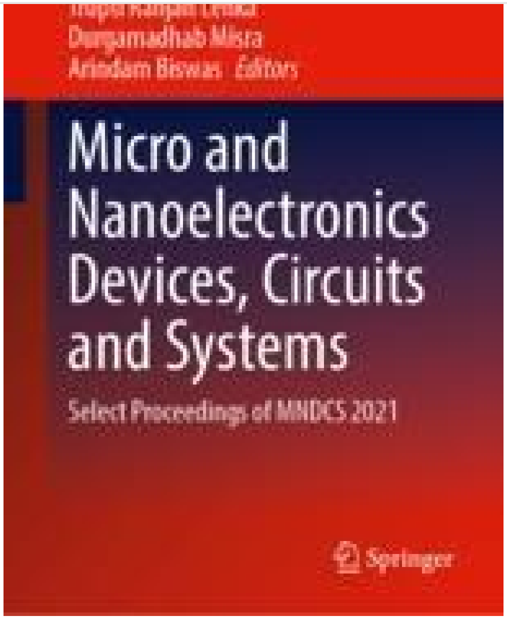

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An Enhanced Sensing Performance with Electrochemical Modulation in ZnO NT based Gas Sensor Devices towards Toxic CO via Foreign Pt Dopant: A Computational Exploration

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Abstract. The design and optimization of high-performance gas sensors is critical for improving industrial safety and environmental monitoring. The present study explores a comparative analysis to draw an understanding of how well pristine zinc oxide (ZnO) nanotubes (NTs), and platinum (Pt)-doped ZnO nanotubes can sense toxic carbon monoxide (CO) gas. The Gaussian 09W program was used to perform first-principles based computations to investigate various electronic properties of the two systems such as CO adsorbed pristine ZnO NT (Type-1), and CO adsorbed Pt-doped ZnO NT (Type-2). Critical factors such as the electron localization function (ELF), binding distance, adsorption energy, Mulliken charge profile, Density of states (DOS), Partial DOS, Fourier Transform Infrared (FTIR) spectra, and several global sensing parameters were evaluated. Cross-interference effect from the surronding was analysed by introducing CO_2 gas in addition to CO (as a mixture of both) for the same devices. Further study was also carried out by examining the interaction at different adsorption sites of the sensing material, and by varying the doping concentration of external platinum (Pt) atom. The interaction between Pt-doped ZnO NT and CO was significantly stronger (-0.7382 eV) than that of the undoped system (-0.2652 eV). Additionally, the Type-2 system demonstrated improved electrical conductivity and enhanced sensitivity. In addition, the obtained ELF mapping indicated stronger molecular interactions in the Pt-doped system. These results confirm Pt-decorated ZnO NTs to be highly reliable and sensitive choices for robust next generation CO gas sensor devices.

Keywords: ZnO nanotube, CO sensing, Pt doping, gas adsorption, ELF, recovery time.

1 Introduction

One of the oldest environmental issues that people have ever encountered is air pollution, which has numerous natural causes. The alarming rise of hazardous gases for the environment and, more specifically, human health, has resulted from the startling industrial progress of recent decades. Of these hazardous gases, carbon monoxide (CO) gas is one of the most dangerous gases affecting both the environment and people. CO is a colorless, odorless, and toxic gas that is produced as a result of partial combustion of organic materials [1]. It accounts for the largest percentage of air pollutants. Its density is 1.145 g/L at 0°C and 1 atm pressure, and its molar mass is 28.01 g/mol. CO being a powerful asphyxiant, is harmful for public health, as it has a high ability to combine with blood hemoglobin, which can have a major impact on respiratory systems, particularly those of humans, and lead to numerous poisoning incidents [2]. The Occupational Safety and Health Administration (OSHA) provides the permissible CO exposure limit to be 50 parts per million (ppm) over an 8-hour cycle [3]. Thus, it is absolutely necessary to detect CO concentrations, in order to safeguard both the environment and humans.

One of the most important steps in reducing environmental pollution is the detection of tiny amount of gas molecules. Zinc oxide (ZnO) nanotubes belong to a prominent class of nanostructures, with significant potential in a large variety of sensing implementation, attributing to their distinctive chemical and physical properties. ZnO NTs are excellent choices for gas sensors and biosensors, due to their high surface-to-volume ratio, chemical stability, and versatile electronic characteristics [4]. ZnO NTs typically exhibit a hollow cylindrical one-dimensional (1D) morphology, offering a substantial surface area, necessary for proper adsorption and interaction with target molecules [5]. The vast surface area, which provides better active sites for interaction, increases their sensitivity. ZnO exhibits a broad bandgap, of approximately 3.37 eV [6]. In sensing applications, this property influences the charge transport parameters. ZnO is a II-VI semiconductor showcasing outstanding optical characteristics [7-8]. At room temperature, it also possesses a binding energy of about 60 meV [9-10]. ZnO nanotubes can potentially be doped with catalytic elements to improve sensitivity and response time, by changing

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