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Performance Analysis of MoS₂ based Gas Sensor Devices Targeting to Detect Different Nitrogen Oxides

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The current study investigates the potential application of pristine molybdenum disulphide (MoS₂), which is a promising member of the transition metal dichalcogenides (TMDs) family, as an effective gas sensing material for the detection of different nitrogen oxides (NO_x) through first-principle-based calculations. From the NO_x family, two gases: nitric oxide (NO, via taking $x = 1$), and nitrogen dioxide (NO₂, via taking $x = 2$) were considered in this study. This paper explored various electronic and structural properties of pristine MoS₂ upon adsorption of NO and NO₂, investigating critical parameters like binding distance, molecular orbital (MOs) energies, electrostatic potential (ESP), density of states (DOS), partial density of states (PDOS) and band structure. Additionally, the electron localization function (ELF) and infrared (IR) spectra were explored to assess the interaction dynamics. The binding distance and HOMO-LUMO (highest occupied molecular orbital – lowest unoccupied molecular orbital) gap indicate the effectiveness of MoS₂ as a sensing material for the detection of different nitrogen oxides, which are hazardous gases causing physical illness and environmental damage. The findings in this research revealed that MoS₂ exhibits higher sensitivity towards NO in comparison to NO₂, as reflected by their respective binding distances 1.68 Å for the NO-adsorbed MoS₂ system, and 1.83 Å for the NO₂-adsorbed MoS₂ system, respectively.

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This is to certify that

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