

Unveiling the Potential of MoSe₂ for Toxic Gas Sensing: Insights from Density Functional Theory and Non-equilibrium Green's Function Calculations

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Abstract : With the rapid development of industrialization and urbanization, air pollution poses significant global environmental challenges, contributing to acid rain, global warming, and adverse health effects. Therefore, it is necessary to monitor the concentration of toxic gases in the atmospheric environment in real-time and to deploy cost-effective gas sensors capable of detecting their emissions. In this study, we systematically investigated the sensing capabilities of the two-dimensional MoSe₂ for seven key environmental gases (NO, NO₂, CO, CO₂, SO₂, SO₃, and O₂) using density functional theory (DFT) and non-equilibrium Green's function (NEGF) calculations. We also investigated the impact of H₂O as an interfering gas. Our results indicate that the MoSe₂ monolayer is thermodynamically stable and exhibits strong gas-sensing capabilities. The calculated adsorption energies indicate that these gases can stably adsorb on MoSe₂, with SO₃ exhibiting the strongest adsorption energy (-0.63 eV). Electronic structure analysis, including projected density of states (PDOS) and Bader charge analysis, demonstrates significant changes in the electronic properties of MoSe₂ upon gas adsorption, affecting its conductivity and sensing performance. We find that oxygen (O₂) adsorption notably influenced the deformation of MoSe₂. To comprehensively understand the potential of MoSe₂ as a gas sensor, we used the NEGF method to assess the electronic transport properties of MoSe₂ under gas adsorption, evaluating current-voltage (I-V), resistance-voltage (R-V) characteristics, and transmission spectra to determine sensitivity, selectivity, and recovery time compared to pristine MoSe₂. Sensitivity, selectivity, and recovery time are analyzed at a bias voltage of 1.7V, showing excellent performance of MoSe₂ in detecting SO₃, among other gases. The pronounced changes in electronic transport behavior induced by SO₃ adsorption confirm MoSe₂'s strong potential as a high-performance gas-sensing material. Overall, this theoretical study provides new insights into the development of high-performance gas sensors, demonstrating the potential of MoSe₂ as a gas-sensing material, particularly for gases like SO₃.

Keywords : density functional theory, gas sensing, MoSe₂, non-equilibrium Green's function, SO

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