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Unveiling the Potential of $MoSe_2$ 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 $MoSe_2$ for seven key environmental gases (NO, NO_2, CO, CO_2, SO_2, SO_3, and O_2) using density functional theory (DFT) and non-equilibrium Green's function (NEGF) calculations. We also investigated the impact of H_2O as an interfering gas. Our results indicate that the $MoSe_2$ monolayer is thermodynamically stable and exhibits strong gas-sensing capabilities. The calculated adsorption energies indicate that these gases can stably adsorb on $MoSe_2$, with SO_3 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 $MoSe_2$ upon gas adsorption, affecting its conductivity and sensing performance. We find that oxygen (O_2) adsorption notably influenced the deformation of $MoSe_2$. To comprehensively understand the potential of $MoSe_2$ as a gas sensor, we used the NEGF method to assess the electronic transport properties of $MoSe_2$ 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 $MoSe_2$. Sensitivity, selectivity, and recovery time are analyzed at a bias voltage of 1.7V, showing excellent performance of $MoSe_2$ in detecting SO_3, among other gases. The pronounced changes in electronic transport behavior induced by SO_3 adsorption confirm $MoSe_2$'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 $MoSe_2$ as a gas-sensing material, particularly for gases like SO_3.

Keywords : density functional theory, gas sensing, $MoSe_2$, non-equilibrium Green's function, SO
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