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“A simulation based study on the selectivity of MoSe₂ for CO and CO₂ gases”

In this paper, we have examined the vital field of gas sensors, which is crucial for environmental monitoring, industrial safety, and healthcare. One of the most important properties of gas sensors is their selectivity, or their capacity to precisely identify and discriminate particular gases in intricate combinations. Selectivity is influenced by a number of important parameters, some of which were brought to light by our inquiry. These include the choice of sensing material, sensing techniques, operating temperature, humidity levels, cross-sensitivity, sensor geometry, gas preconcentration methods, and the usage of sensor arrays. Additionally, we covered a number of physical and chemical processes, including adsorption and desorption, conductivity changes, capacitance variations, optical absorption, mass loading, chemical reactions, heat production or consumption, ionisation, gas diffusion, and changes in mechanical properties that support gas sensor operations. This study used the gas diffusion method and a variety of sensing materials to evaluate the performance of the MoSe₂. We observed distinct surface concentration levels in response to CO and CO₂ gases on the active surfaces of MoSe₂ through simulations. On the other hand, MoSe₂ responded better to CO₂ than to CO. Our results highlight the significance of customising sensor choices based on individual gas detection requirements. As a result, this study clarifies the crucial variables affecting gas sensor selectivity and offers insightful information about the gas-sensing capacities of MoSe₂. Additionally, it highlights the potential uses.

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