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Defect Engineering in 2D Materials for Enhanced Chemical Sensing

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This research focuses on the enhancement of two-dimensional (2D) materials such as graphene, transition metal dichalcogenides (TMDs), and MXenes for advanced sensor applications. These materials are celebrated for their ability to detect specific analytes and respond to physical stimuli, making them ideal for a variety of detection strategies in fields ranging from environmental monitoring to medical diagnostics. Despite their known sensitivity and responsiveness to various stimuli, these materials face challenges in selectivity and sensitivity due to interference and noise. This study aims to computationally investigate the impact of engineered defects, specifically substitution and vacancy defects, on the sensing properties of these materials. By applying Density Functional Theory (DFT) within the Quantum Espresso software, our study models the interaction of defected 2D materials with impurities in the environment such as volatile organic compounds (VOCs), gaseous molecules such as NH3, and CO2. The research will explore how these defects, including doping of the lattice with elements like boron, nitrogen and creation of vacancy sites, enhance adsorption and charge transfer processes. Our findings aim to significantly improve the performance of sensors by increasing their sensitivity and selectivity, potentially revolutionizing industries such as public health and safety, environmental monitoring, and biotechnology. The outcomes will also provide deeper insights into the fundamental properties of 2D materials interacting with complex molecular systems, potentially opening new avenues for their use in advanced sensor and quantum technologies.

Keyword-1

Chemical sensing

Keyword-2

Defect engineering

Keyword-3

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