SUMMARY

Hydrogen sulfide (H_2S) and sulfur dioxide (SO_2) are toxic gases that pose serious threats to human health and the environment, thus requiring rapid, sensitive, and selective detection. Graphene offers excellent electrical conductivity and good mechanical stability, yet its relatively weak interaction with gas molecules limits its sensing performance. To address this limitation, a graphene/hexagonal boron nitride (G/h-BN) heterostructure has been developed, offering enhanced mechanical stability and improved electronic properties. This study employs *Density Functional Theory* (DFT) computational modelling to evaluate the sensing capabilities of G/h-BN, both in its pristine form and with engineered atomic vacancies of boron (B) and nitrogen (N), for the detection of H_2S and SO_2.

The research was conducted entirely through computational simulations using the *Quantum ESPRESSO* package with a *plane-wave* basis set and *pseudopotentials*. The modelled systems included pristine graphene, pristine G/h-BN, and G/h-BN with B and N atomic vacancies. Simulations involved structural optimisation, adsorption energy calculations, *Density of States* (DOS) analysis, *work function* evaluation, and estimation of gas recovery times. H_2S and SO_2 molecules were modelled in various adsorption orientations to identify the most stable configurations. The resulting data were analysed to assess the influence of the h-BN layer and crystal defects on the mechanical, electronic, and sensing performance of the systems.

Simulation results reveal that G/h-BN exhibits stable interlayer interactions with an energy of –0.75 eV, accompanied by an increase in the work function from 4.42 eV to 4.59 eV. The presence of the h-BN layer slightly increases adsorption energy (~0.01 eV) and significantly accelerates recovery times (0.3 fs for H_2S and 0.001 fs for SO_2), although at the expense of mechanical strength. B-vacancy defects improve both mechanical strength and adsorption capacity for H_2S, whereas N-vacancy defects enhance selectivity for SO_2 but reduce mechanical robustness. Changes in the DOS profiles caused by these defects demonstrate that structural engineering can improve both sensitivity and selectivity. Overall, G/h-BN with engineered atomic vacancies presents an efficient and promising gas-sensing platform for the detection of H_2S and SO_2.