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Comparative Study between Pristine MoS₂ and Rh-Doped MoS₂ based 2D TMDs for Identifying the Presence of SO₂ Gas

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This paper explores enhancement into the gas-sensing capabilities of Rhodium (Rh)-doped molybdenum disulfide (MoS₂) sheet over pristine MoS₂ sheet towards sulfur dioxide (SO₂) gas identification, which is a toxic air pollutant. The investigation was performed through first-principles-based computational methods using tools such as Gaussian 09W, GaussView 6.0, and Material Studio for modelling and analysis of the SO₂ gas adsorption on pristine and Rh-doped MoS₂ sheets. In this current study, several critical electrochemical properties such as the molecular orbitals (MOs), molecular electrostatic potential (MEP), density of states (DOS), projected density of states (PDOS), band structure, infrared (IR) spectra, and electron localization function (ELF) were studied. It has been observed from the above-mentioned parameters that Rh doping increased the reactivity as well as enhanced the sensitivity of pristine MoS₂ sheet considerably towards SO₂. The HOMO-LUMO (highest occupied molecular orbital-lowest unoccupied molecular orbital) gap was found to increase in the case of Rh-doped MoS₂ system, depicting higher kinetic stability compared to pristine MoS₂ system. Rh-doped MoS₂ sheet depicted significant adsorption with a stronger adsorption energy of -0.816 eV as well as smaller binding distance of 2.099 Å as compared to pristine MoS₂ sheet for the SO₂ gas molecule. These observations showed that the introduction of Rh atom into the pristine MoS₂ sheet enhanced the interaction of the sensing material with SO₂ gas, which in turn give better sensing performance. Thus, it can be said that the Rh-doped MoS₂ sheet can be used as an effective sensing material for SO₂ gas detection.

CERTIFICATE FOR ORAL PRESENTATION

This is to certify that
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