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| Title: | Enhanced sensitivity of band gap engineered phosphorene towards NH3 and NO2 toxic gases |
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| Abstract: | Band gap tuning is an efficient approach to modify the sensing ability of phosphorene. Herein, density functional theory (DFT) calculations have been performed to investigate the effect of various group elements (III-VI) doping in phosphorene sheet for NH3 and NO2 gas sensing ability. The presence of NH3 and NO2 gas molecules on doped phosphorene nanosheet is found to alter the structural network, electronic properties hence leading to a better sensing and selectivity of the doped nanosheet. B doped phosphorene showed maximum adsorption of −2.64 eV and −3.70 eV towards the NH3 and NO2 gas molecules respectively. NH3 adsorption on C, Si and S-doped phosphorene causes direct to indirect band gap transition while NO2 adsorption shows indirect band gap for pristine and S-doped phosphorene. Simulated scanning tunneling microscopy (STM) images showed different structural phases after gas adsorption due to electronic hybridization with orbitals from the upmost phosphorous atoms and the gas molecule. After gas adsorption, some flat bands are observed and localized states appear near the Fermi level, which are readily accessible at low bias voltages, thereby indicating the improved sensory functionality of doped phosphorene. |
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