Band gap engineering of phosphorene for gas sensing properties

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Abstract

Sensors with superior sensitivity and selectivity are of great concern for the detection of toxic gases which are highly related to human health and environments. Herein, phosphorene as a promising sensing 2D material has been studied due to their high specific area and the associated charge transfer between gas molecules and the former [1,2]. First-principles density functional theory (DFT) has been adopted to study the effect of B, C and S doping in phosphorene sheet on NO_2 adsorption. A double-ℨ polarized basis set within generalised gradient approximations (GGA) approach for Perdue-Burke Ernzerhof (PBE) [2] exchange-correlations was used. The structural optimization was done until the force acting on each atom is less than 0.01 eV/A°. Electronic properties were investigated in terms of band structure of the pristine and doped phosphorene after NO_2 adsorption as shown in figure 1. Presence of NO_2 introduces some localized states in pristine phosphorene and doped phosphorene. After NO_2 molecule adsorption B doped phosphorene shows metallic features while C and S reduces the band gap. Adsorption energy also increases implying NO_2 binds strongly with doped phosphorene. This generally indicates a prompted interaction upon substitution. Owing to puckered surface which intrinsically provides more adsorption sites and possesses a high surface-volume ratio, hence doped phosphorene should be ideal for gas sensing and capturing.

References

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Figure

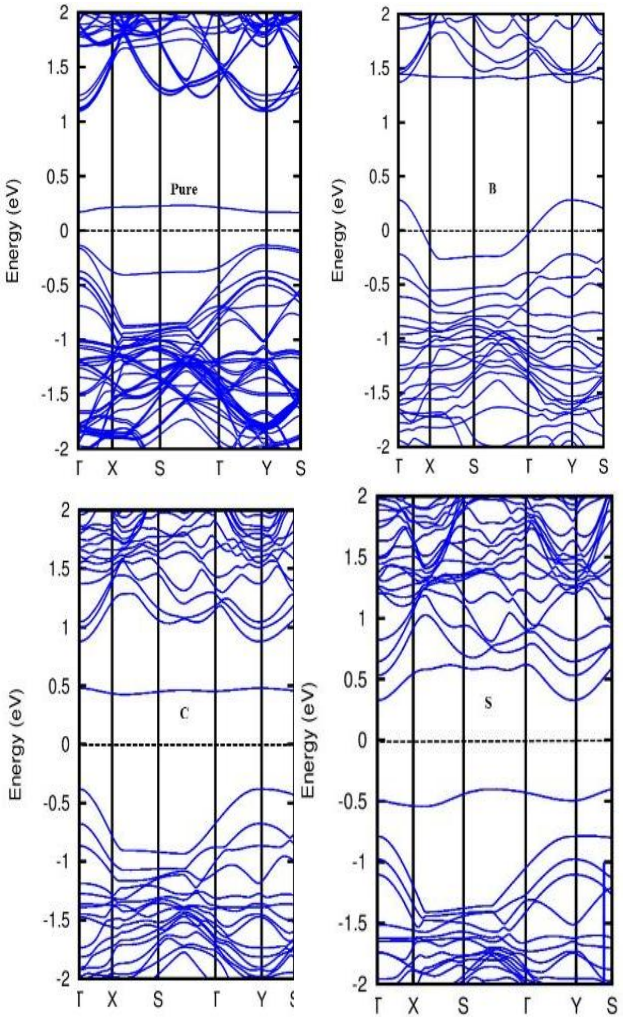

Figure 1: Plots of band structure for pristine, B, C and S after NO_2 adsorption