Gaganpreet
Prateek Ahuja
P. Balanarayan
Indian Institute of Science Education and Research, Knowledge city, Sector 81, SAS Nagar, Manauli PO 140306 Mohali, India

gaganpreet@iisermohali.ac.in

Doped phosphorene nanosheet based gas sensor: an application to NH_3

Abstract

Sensing toxic gases is crucial in monitoring and controlling environmental pollution and has applications in medical and agricultural applications. Gas sensing technology is mainly based on the variation of electrical properties and anomalous effects in optical, mechanical, thermal and chemical properties. The discovery of two-dimensional (2D) layered materials offers a novel platform for electricalconductance-based nanoscale gas sensors due to their superior sensitivity/selectivity and relatively low cost over their bulk counterparts. These materials exhibit outstanding mechanical performance as demonstrated in the studies of dichalogenides (MOS_2 and WeS_2 etc.),graphene, silicone and so on [1-4]. However, these materials exhibit certain intrinsic shortcomings such as low carrier mobility asin MOS_2 [5], lack of band gap in graphene to turn off the electric current [6] which has prompted researchers to explore new layered materials. Recently, a new class of layered phosphorene [7,8] material has proven to be a promising gas sensor due to its large specific area and the associated charge transfer between gas molecules and the former. Black phosphorene is the most stable allotrope resembling graphite in its structure, where the adjacent layers are held together by the weak van der Waals' attractive forces. In a phosphorene monolayer, each phosphorus atom forms bonds with three adjacent phosphorus atoms in a puckered honeycomb structure. Phosphorene shows good sensing functionality with better performance than graphene and MOS_2 [9,10]. Thus, tuning of its natural band gap by various group elements allows [11] it for great flexibility in the design and optimization of electronic, opto electronic devices and sensing properties. In this work, we report the chemical sensing of ammonia. First-principles density functional theory (DFT) has been adopted to studytheeffect of substitutional doping of group elements (III, V) in phosphorene sheet on NH_3adsorption. The DFT calculations using the Perdew-Burke-Ernzerhof (PBE) variant of the generalized gradient approximation (GGA) for the Exchange correlation functional, has been performed. Doping of the phosphorene sheet has been modelled in a periodicslab geometry by considering a series of 3X3 supercells with one phosphorous atom replaced by the dopant atom, thereby leading to a dopant concentration of 3.125%. Nature of the gas adsorption has been investigated by studying the roles of charge transfer between the host layer and gas molecule and the effect of adsorptionon the structural and electronic properties of the host layers. The adsorption of a NH_3 molecule on doped phosphorene nanosheet is found to alter the structure of doped nanosheet, as shown in the figure given. Furthermore, in the band structure plots, dopants have been observed to induce some localized states near the Fermi level, which are readily accessible at low bias voltages, thereby indicating the sensory functionality of doped phosphorene.

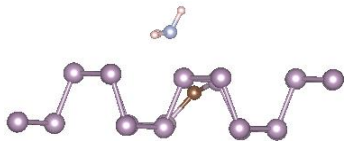

Figure 1: NH_3 molecules placed over B doped phosphorene.

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