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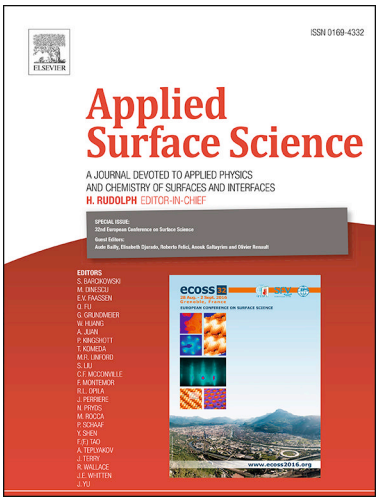

Full Length Article

Adsorption of the NH_3, NO, NO_2, CO_2, and CO Gas Molecules on Blue Phosphorene: A First-Principles Study

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Adsorption of the NH_3, NO, NO_2, CO_2, and CO Gas Molecules on Blue Phosphorene: A First-Principles Study

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***Abstract*—We report on a first-principles study of the electronic and transport properties of pristine, B-, C-, N-, O-doped blue phosphorene (BlueP) with the adsorption of gas molecules NH_3, NO, NO_2, CO, and CO_2. The adsorption distances, adsorption energies, charge transfer, density of states (DOS) and transmission spectra of these gas molecules on molecules on doped as well as undoped BlueP is systematically investigated in this work. Our calculations show that the adsorption energy of NO and NO_2 on pristine BlueP is the largest among the considered gas molecules, suggesting that pristine BlueP is more sensitive to these two gases. The results indicate that the pristine BlueP exhibits a weak sensitivity to NH_3 and CO molecules, while B-doped BlueP strongly adsorbs NH_3 and CO by way of strong chemical bonds. C-doped BlueP can enhance the sensitivity to NH_3 gas molecules. The current-voltage (I-V) characteristics of the sensors are calculated using non-equilibrium the Green's function (NEGF) formalism. Theses sensors show characteristic responses along both the zigzag and the armchair directions depending on the type of the gas molecules.**

Keywords—blue phosphorene; gas sensor; first-principles; NEGF

I. INTRODUCTION

Sensing toxic gas molecules is critical in environmental pollution monitoring, control of chemical processes, and agricultural and medical applications [1]. Two-dimensional (2D) materials offer great potential applications for gas sensing due to their unique properties and large surface-to-volume ratio [2]. Phosphorene, a new 2D material, has recently been exfoliated by mechanical cleavage of black phosphorus, the most stable allotrope of the element phosphorus in ambient condition [3]. The high hole carrier mobility and direct band gap of phosphorene promise new applications in electronics and optoelectronics [4–11]. First-principles calculations indicate that adsorption of gas molecules such as NO_2, NO, NH_3 and SO_2 induces appreciable variations to the electronic and transport properties of phosphorene [12–18], revealing the promising sensing capability of this 2D material. Blue phosphorus, a new allotrope of phosphorus, was first predicted by Zhu et al. in 2014 [19], and a molecular-beam epitaxial growth of its single layer on Au(111) has been reported by Zhang et al. in 2016 [20]. It is an indirect gap semiconductor with the band gap of about 2eV [19]. Theoretical studies have been carried out to investigate the interactions of blue phosphorene (BlueP) with different molecules [21–23], however, the effect of such molecules on transport properties of BlueP is still lacking.