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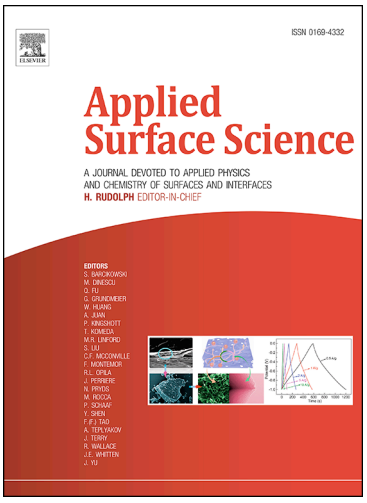

Full Length Article

Hydrogen adsorption on alkali metal decorated blue phosphorene nanosheets

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Hydrogen adsorption on alkali metal decorated blue phosphorene nanosheets

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Abstract: Hydrogen storage capabilities of blue phosphorene nanosheet, decorated with lithium and sodium atoms were systematically studied using *ab-initio* Density Functional (DFT) calculations. Hydrogen molecule adsorbs on pristine blue phosphorene with an adsorption energy of 0.06 eV, which is much lower than the threshold energy of ~0.10eV required for practical applications. When blue phosphorene is decorated with lithium or sodium atoms on its surface, hydrogen adsorption energies are drastically increased to 0.25eV and 0.18eV respectively. It is found that a lithium atom adsorbs up to three and sodium atom up to four hydrogen molecules. Analysis of density of states and difference charge density calculations confirm the hybridization of hydrogen and lithium states. Coverage studies show a gravimetric storage capacity for hydrogen to be 5.5% on lithium decorated blue phosphorene, which is better than that of lithium decorated black phosphorene (4.4%).

Keywords: Surface Adsorption; Adsorption Energy; Hydrogen Storage; Surface Coverage; DFT; van der Waals interaction

1. Introduction

Two dimensional (2D) layered materials like graphene, silicene, germanene, transition metal di-chalcogenides, hexagonal boron nitride, layered metal halides etc., have emerged as highly promising materials for a variety of applications. Due to their extraordinary mechanical, electronic, and optical properties [1-4], these applications lie across diverse area like nanoelectronics, photonics and device physics. Phosphorus is an element that is abundant, in the form of three well-known allotropes, red, white, and black phosphorus [5,6]. Black phosphorus[7]