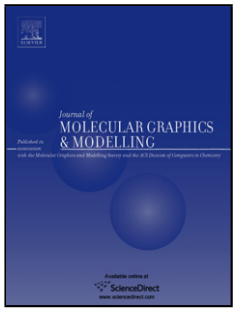

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<AT>Sensing properties of monolayer borophane nanosheet towards alcohol vapors: a first-principles study

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<ABS-Head><ABS-HEAD>Graphical abstract
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<ABS-P><xps:span class="xps_Image">fx1</xps:span>

<ABS-HEAD>Highlights► The adsorption behavior of alcohol on borophane nanosheet is studied. ► The favorable adsorption sites of alcohol on borophane nanosheet are identified. ► The borophane nanosheets are highly sensitive towards alcohol vapors. ► The monolayer borophane sheets can be used to detect alcohol vapors.
<ABS-HEAD>ABSTRACT
<ABS-P>The electronic properties of borophane and adsorption behavior of three distinct alcohol vapors namely methanol, ethanol and 1-propanol on borophane nanosheet is studied using DFT method for the first time. The state-of-the-art provides insights on to the development of new two dimensional materials with the surface passivation on boron nanostructures. The DOS spectrum provides clearer vision on the electronic properties of borophane nanosheet. The monolayer of borophane gives rise to the opening of band gap, which can be used for the detection for volatile organic vapors. The adsorption properties of alcohol vapors on borophane base material are analyzed in terms of Mulliken charge transfer, average energy gap variation, adsorption energy and HOMO-LUMO gap. The most suitable adsorption sites of methanol, ethanol and 1-propanol molecules on borophane nanosheet are investigated in atomistic level. The adsorption of alcohol molecules on borophane nanosheet is found to be more favorable. The findings suggest that the monolayer borophane nanosheet can be utilized to detect the presence of alcohol vapors in the atmosphere.
<KWD>Keywords: borophane; nanosheet; alcohol; formation energy; adsorption; energy gap

<H1>1. Introduction

Graphene, as a habitual Dirac cone material exhibits spintronics and electronic properties [1] such as high carrier mobility [2], ballistic charge transport [3] and quantum Hall effects [4]. Its