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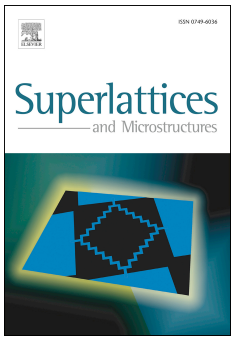

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The role of boron nitride nanotube as a new chemical sensor and potential reservoir for hydrogen halides environmental pollutants

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Abstract

Density functional theory (DFT) studies on the interaction of hydrogen halides (HX) environmental pollutants and the boron nitride nanotubes (BNNTs) have been reported. To exploit the possibility of BNNTs as gas sensors, the adsorption of hydrogen fluoride (HF), hydrogen chloride (HCl) and hydrogen bromide (HBr) on the side wall of armchair (5,5) boron nitride nanotubes have been investigated. B3LYP/6-31G (d) level were used to analyze the structural and electronic properties of investigate sensor. The adsorption process were interpreted by highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO), quantum theory of atoms in molecules (QTAIM), natural bond orbital (NBO) and molecular electrostatic potential (MEP) analysis. Topological parameters of bond critical points have been used to calculate as measure of hydrogen bond (HB) strength. Stronger binding energy, larger charge transfer and charge density illustrate that HF gas possesses chemisorbed adsorption process. The obtained results also show the strongest HB in HF/BNNT complex. We expect that results could provide helpful information for the design of new BNNTs based sensing devices.

Keywords: chemical sensor; boron nitride nanotube; hydrogen halides; DFT.

1. Introduction

Pristine boron nitride nanotubes (BNNTs) were theoretical predicted in 1994 by Rubio et. all [1] and experimentally synthesis in 1995 by Chopra et. all [2]. Since then various promising applications of BNNTs have inspired broad researches in the field of nanotechnology [3, 4]. BNNTs consist co-axial hexagonal boron-nitride network. BNNTs with a Young's moduls of