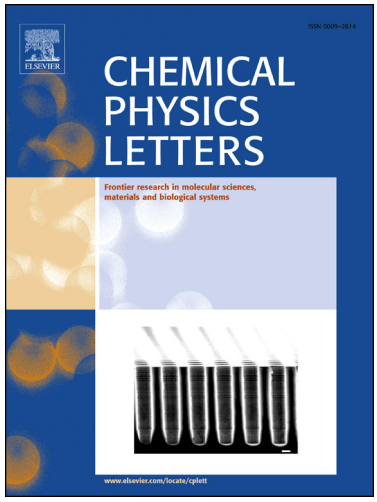

Research paper

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Studying the effects of the configuration of doped Al atoms on the conductive properties of boron nitride nanotube using density functional theory

Zahra Tavangar[1,2,1], Masood Hamadanian[1,2] Hadi Basharnavaz[1]

[1]*Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, Iran.*

[2]*Institute of Nano Science and Nano Technology, University of Kashan, Kashan, Iran.*

Abstract

In this paper, we study the effects of the configuration of two Al atoms doped into the unit cell of (7, 0) BNNTs, on their structural and electronic properties in solid state using density functional theory methods. Also, all possible configurations for Al double doped (7, 0) BNNT were investigated. The results showed that with Al doping, band gap decreased. Furthermore, an impurity state appears near the Fermi level when two Al atoms replace two boron atoms of adjacent layers. Contour plots of charge density distribution showed a protuberance surrounding N and B atoms adjacent to the substitute Al atoms.

Keywords: 2×Al doped boron nitride nanotube, Configuration, Electronic properties, Density functional theory, Fermi energy level.

Introduction

[1]Corresponding author. Tel.: +98 31 55912366; fax: +98 31 55912397.
E-mail address: z.tavangar@kashanu.ac.ir (Z. Tavangar).