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Dorsa S. Fartab, Amirhossein Ahmadkhan Kordbacheh

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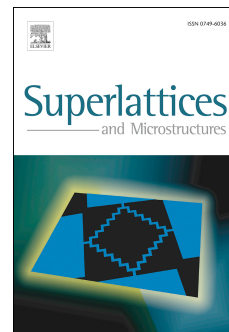
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Lithium doping and vacancy effects on the structural, electronic and magnetic properties of hexagonal boron nitride sheet: A first-principles calculation

Dorsa S Fartab and Amirhossein Ahmadkhan Kordbacheh

Materials Simulation Laboratory, Department of Physics, Iran University of Science and Technology, 1684613114 Tehran, Iran

E-mail: akordbacheh@iust.ac.ir

Abstract. The first-principles calculations based on spin-polarized density functional theory is carried out to investigate the structural, electronic and magnetic properties of a hexagonal boron nitride sheet (h-BNS) doped by one or two lithium atom(s). Moreover, a vacancy in the neighborhood of one Li-substituted atom is introduced into the system. All optimized structures indicate significant local deformations with Li atom(s) protruded to the exterior of the sheet. The defects considered at N site are energetically more favorable than their counterpart structures at B site. The spin-polarized impurity states appear within the bandgap region of the pristine h-BNS, which lead to a spontaneous magnetization with the largest magnetic moments of about $2 \mu_B$ in where a single or two B atom(s) are replaced by Li atom(s). Furthermore, the Li substitution for a single B atom increases the density of holes compared to that of electrons forming a p-type semiconductor. More interestingly, the structure in which two Li are substituted two neighboring B atoms appears to show desired half-metallic behavior that may be applicable in spintronic. The results provide a way to enhance the conductivity and magnetism of the pristine h-BNS for potential applications in BN-based nanoscale devices.

Keywords: Hexagonal boron nitride, Lithium doping, Vacancy, First-principles

1. Introduction

Boron nitride (BN) is the lightest chemical compound of Group III –V with equal numbers of boron and nitrogen atoms. It has been synthesized in amorphous (a-BN) and various crystalline structures. Hexagonal boron nitride also called as h-BN, α -BN and g-BN, is the most stable crystalline form at room temperature. h-BN is attractive due to its interesting potential applications such as lubricants, protective coatings and deep-ultraviolet light emitter. Moreover, it is applied as a dielectric layer in electronics and acts as a carrier catalyst [1-5]. h-BN is a graphite-like layered material, in which C atoms are substituted with alternating B and N atoms. Within each layer, due to the electronegativity difference between B and N atoms, the charge distribution is biased towards N atom to form a strong ionic and covalent bond, while weak van der waals interactions exist between adjacent layers [6-8]. Following the synthetization of single sheets of graphite (graphene), and the discovery of its singular properties, research interests have been attracted to analogous two-dimensional structures. The single

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