Structural, electronic and magnetic properties of carbon doped boron nitride nanowire: *Ab initio* study

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ABSTRACT

Using spin-polarized density functional theory calculations, we demonstrated that carbon doped boron nitride nanowire (C-doped BNNW) has diverse electronic and magnetic properties depending on position of carbon atoms and their percentages. Our results show that only when one carbon atom is situated on the edge of the nanowire, C-doped BNNW is transformed into half-metal. The calculated electronic structure of the C-doped BNNW suggests that doping carbon can induce localized edge states around the Fermi level, and the interaction among localized edge states leads to semiconductor to half-metal transition. Overall, the bond reconstruction causes of appearance of different electronic behavior such as semiconducting, half-metallicity, nonmagnetic metallic, and ferromagnetic metallic characters. The formation energy of the system shows that when a C atom is doped on surface boron site, system is more stable than the other positions of carbon impurity. Our calculations show that C-doped BNNW may offer unique opportunities for developing nanoscale spintronic materials.

1. Introduction

One and two dimensional (1D and 2D) nanostructures materials, such as nanotubes (NTs), nanowires (NWs) and graphene-like materials have attracted great interest over the past decade due to their unique physical and chemical properties and potential application in the fabrication of nanoscale electronic, photonic and sensing devices [1,2]. The three-component boron-nitrogen-carbon (BN-C) system has been subjected to much attention, owing to BN-C nanostructures having predicted higher chemical and thermal stabilities than those of carbon nanostructures [3]. Electronic properties of these hybrid structures have been studied by many theoretical and experimental groups [4–6]. Guo et al. by using density functional calculations investigated spin polarization of the injected carriers in C-doped BN nanotubes [7]. They found that BN nanotube can be a ferromagnet due to C atom doping. Also, Huang et al. studied half-metallicity behavior of BN-C nanotubes and showed that electronic and magnetic properties of BN-C nanotubes are dependent on position and concentration of carbon atoms [8]. BN nanotubes and BN nanowires are electrically insulating with a band gap about 5–6 eV independent of their morphologies and structures [9,10], while CNTs are metallic or narrow-band gap semiconducting depending on their chirality, and graphene is a semimetal with zero band gap [11]. Nearly hybrid structures of BN and C systems make it possible to construct hybrid ternary BN-C honeycomb lattices and corresponding BN-C nanostructures with electrical properties intermediate between those of pure BN and C systems [12–15]. Recently, Wei et al. utilized experimental technique synthesized C-doped BN nanotubes, nanosheet and nanoribbon [16]. Researches show that synthesis and characterization of BNC nanostructures such as nanotube, nanowire and nanosheet are possible [17]. Also, Duan et. al studied fluorine doped graphene monolayer to achieve better sensing properties of graphene by changing in electronic structure of graphene [18]. They showed that depending on the fluorine binding sites, the valence band can serve as a valence band or a conduction band.

There are some experimental articles for BN-C nanowire, but there are not any theoretical or computational articles about nanowire structure. Because of this reason, the electronic and magnetic properties of pristine and C-doped BN nanowire are studied by the full potential linear augmented plane waves plus local orbital in the framework of the density functional theory. All possible configurations for doping one and two carbon atoms doping are considered too. Some obtained results are similar with the other computational data for BN-C nanotube. The present calculations can be helpful for manufacturing nanoscale spintronic devices.

2. Computational details

In this work, the electronic and magnetic properties of pristine and carbon doped BN nanowire are investigated by the full potential augmented plane wave plus local orbital (FPAPW+lo) in the framework of the density functional theory [19] as implemented WIEN2k package [20]. For calculating energy band gap of BN bulk the generalized gradient approximation with the Pedrew-Bruke-Ernezerhof [21], Engel-Vosko [22] and modified Becke-Johanson (mBJ) [23] are used to describe the exchange-correlation term. The obtained results show that the bulk energy gap of boron nitirde for mBJ functional [24] are good agreement with experimental data [23]. So, the density of states of BN nanowire are calculated by GGA-PBE and mBJ-GGA functionals. The basis quality, measured by the product $R_{MT}K_{max}$ (R_{MT} – minimal atomic sphere radius and K_{max} – length of maximal reciprocal lattice vector) is set to 7. The supercell is large enough to ensure that the vacuum space is at least 12 Åto avoid the interaction between periodic images. Charge is converged at 10^{-4} e, and the residual force on all atoms is converged to below 0.01 eV/Å. A total of 300 k-point is used to sample the Brillouin zone [25].
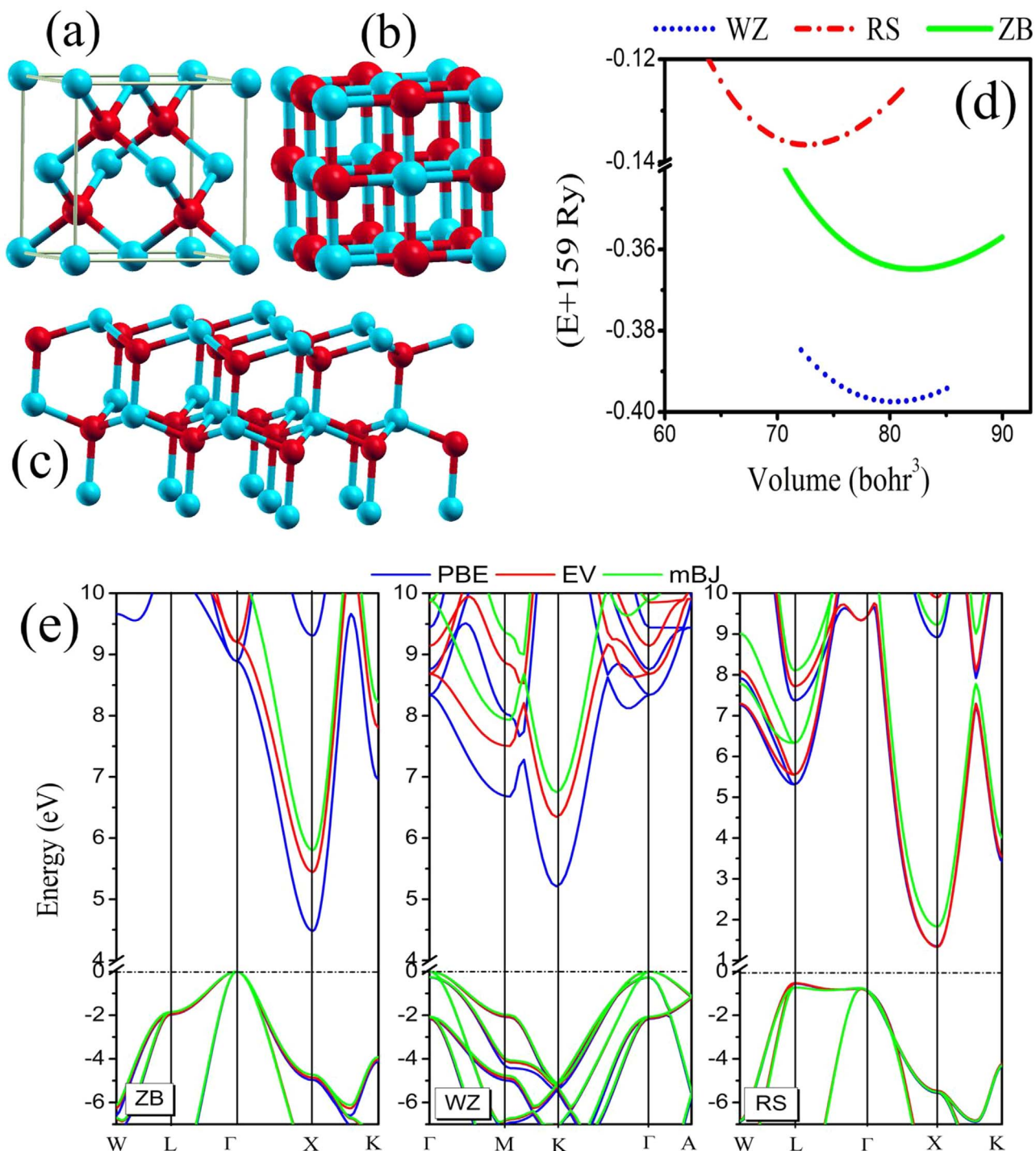
Fig. 1. Crystal structures of BN bulk a) zinc-blende, b) rock-salt and c) wurtzite. d) energy (Ry) versus volume (bohr^3) for these phases of BN. The curves are obtained using the third-order Birch-Murnaghan equation of states. e) The energy band structure of zinc-blende, rock-salt and wurtzite structures by GGA-PBE, EV and mBJ methods.