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Structural, electronic and magnetic properties of C atom doped AlN nanoribbons

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ABSTRACT

First-principles calculations are performed to study the structural, electronic and magnetic properties of pure and C atom doped AlN nanoribbons with both zigzag edge (ZAlNNR) and armchair edge (AAlNNR). With the substitution of one N (Al) atom by a single C atom, a local expansion (a local contraction) takes place, and the C atom is preferred to substituting an edge N or Al atom in 7-ZAlNNR or 7-AAlNNR. Furthermore, by substituting C atom at different positions, the systems may turn into magnetic semiconductors or show a metallic character, which may open a way to design magnetic nanodevices based on AlNNR.

1. Introduction

With the successful research and application of grapheme nanoribbons (GNRs), the graphitic-like planar structures have attracted much attention. Early in 2003, the AlN nanoribbons (AlNNRs) with hexagonal structure have been successfully synthesized by evaporating aluminum powder in ammonia/nitrogen atmosphere at 1200 °C [1]. As an important member of group III nitrides, AlN has a wide direct bandgap of 6.2 eV, and is characterized by its superior properties such as high melting point, excellent thermal conductivity, high resistance to chemicals, and reliable dielectric properties [2,3], therefore is widely used in today's electronics industry. Due to the large iconicity of the Al–N bond, AlNNRs may possess novel properties different from GNRs, leading to new potential applications in optics and nanoscale electronic devices [4].

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With the development of synthesizing techniques, doping AlNNRs with other elements to obtain specific performance is become possible. Previous studies of AlNNRs have shown that AlNNRs are semiconducting and nonmagnetic. In order to obtain magnetic semiconductor, the traditional method is substituting AlNNRs with a magnetic transition metal such as Cr, Mn, Fe, Co and Ni. But the Curie temperatures of these systems are below room temperature, which means that it is difficult to put them into practice. So an effective way to overcome the drawback is to dope the AlNNRs with non-metal elements. In fact, there are many studies which have reported that nonmetal elements induce magnetic behavior both experimentally and theoretically [5–14]. Therefore, the studies of C atom doped AlNNRs have theoretical basis and practical significance.

In present paper, the structural, electronic and magnetic properties of pure AlNNR and C-doped AlNNR with either zigzag edge (ZAlNNR) or armchair edge (AAlNNR) have been investigated systemically by using the first-principles methods. The rest of the paper is organized as follows. In the second section, the structure model and calculation method are described in detail. The calculated results and discussions are given in the third section. The last section is devoted to the conclusions.

2. The calculation method and model

As is shown in Fig. 1, the monolayer hexagonal AlN nanoribbons consist of alternating N and Al atoms with each inner N (Al) atom having three Al (N) atoms as its neighbors. However, for N (Al) atoms at two edges, there are only two Al (N) atoms as their nearest neighbors. In order to eliminate the dangling bond, we attach H atoms to each edged N (Al) atoms. The optimized geometry structures for (a) 7-ZAlNNR and (b) 7-AAlNNR with H atoms terminated at both edges are shown in Fig. 1 as examples. The blue, purple and white balls represent N, Al and H atoms, respectively. The ZAlNNR's width is definited by the number of the zigzag chains (N_z) across the ribbon width. Thus we refer to a ZAlNNR with N_z chains as N_z-ZAlNNR. Likewise, the width of AAlNNR is classified by the number of dimer lines (N_a) across the ribbon width, a AAlNNR with N_a chains is called N_a-AAlNNR.

Calculations are performed by using the Vienna ab initio simulation package (VASP) based on DFT [15–18]. The electron–ionic core interaction is represented by the PAW potentials [19], which are more accurate than the ultrasoft pseudopotentials. In order to treat electron exchange and correlation, we choose the Perdew–Burke–Ernzerhof (PBE) [20] formulation of the GGA, which yields the correct ground-state structure of the combined systems. The plane-wave cutoff energy is chosen to be 450 eV. In order to present artificial inter-ribbon interactions, individual AlNNRs are separated by a sufficiently large vacuum space, the edge-to-edge distance and the layer-to-layer distance are taken to be 15 Å. The $2s^2sp^3$, $3s^23p^1$, $2s^2p^2$ and $1s^1$ electrons are taken as the valence electrons for N, Al, C

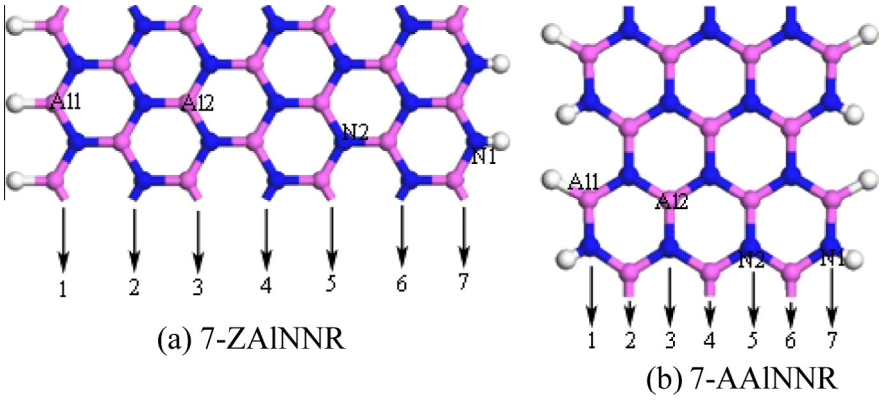

Fig. 1. The optimized geometry structures of: (a) 7-ZAlNNR and (b) 7-AAlNNR with H atoms terminated at both edges. The blue, purple and white balls represent N, Al and H atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)