Density functional study of manganese atom adsorption on hydrogen-terminated armchair boron nitride nanoribbons

ABSTRACT

In this paper, we have investigated stable structural, electric and magnetic properties of manganese (Mn) atom adsorption on armchair hydrogen edge-terminated boron nitride nanoribbon (A-BNNRs) using first principles method based on density-functional theory with the generalized gradient approximation. Calculation shows that Mn atom situated on the ribbons of A-BNNRs is the most stable configuration, where the bonding is more pronounced. The projected density of states (PDOS) of the favored configuration has also been computed. It has been found that the covalent bonding of boron (B), nitrogen (N) and Mn is mainly contributed by s, d like-orbitals of Mn and partially occupied by the 2p like-orbital of N. The difference in energy between the inner and the edge adsorption sites of A-BNNRs shows that Mn atoms prefer to concentrate at the edge sites. The electronic structures of the various configurations are wide, narrow-gap semiconducting and half-metallic, and the magnetic moment of Mn atoms are well preserved in all considered configurations. This has shown that the boron nitride (BN) sheet covered with Mn atoms demonstrates additional information on its usefulness in future spintronics, molecular magnet and nanoelectronics devices.

Keyword: Boron nitride nanoribbons; Density functional theory; Structural; Electric and magnetic properties