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AB initio and DFT study of energetic, stability, and nuclear magnetic resonance of BN nanotube

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Inorganic nanotubes like BN are very interesting due to their unparalleled structure and properties [1, 2]. In comparison with CNTs, BNNTs are more chemically and thermally stable and their electronic behavior is completely different from CNTs which caused BNTs to become more desirable for usage in nano devices, manufacturing and also high temperature environments [3, 4]. All BN nanotubes have wide band gap semiconductor properties about 5.5 eV [5-7]. Geometry optimization, stabilities and nuclear magnetic resonance parameters of BN armchair nanotubes were carried out by ab initio and different levels of DFT methods (B3LYP, B1LYP, B3PW91, B1P86 and LSDA) by using 6-31g (d) basis sets implemented in Gaussian 03 program to perform its application as a trace and the base of functionalizing in drug deliveries system. The calculations were done on armchair model of BN (4, 4) nanotubes which consist of 16 atoms of B, 16 atoms of N and 16 atoms of hydrogen. Geometric optimization of the nanootube carried out by the B3LYP method and 6-31G basis set. The energy gap of this nano semiconductor and the thermodynamic properties of nano semiconductor were reported. In addition, the chemical shielding (CS) tensors, isotropic and anisotropic tensors and asymmetric parameters of 15N and 11B nuclei are calculated which are sensitive to electronic density and also have shown important points to electrostatic properties of BN nanotubes. Comparison between different NMR values at different levels of DFT theory and ab initio method were done to evaluate the 15N and 11B NMR parameters.

Biography

Elham pournamdari has completed her PhD at the age of 31 years from science and research branch, Islamic Azad University. She is the chemistry director of Islamshahr branch of Islamic Azad university. Her research mostly focused on inorganic and calculational chemistry of inorganic molecules and nonostructures. She has published more than 10 papers in journals and participated more than 5 confrences.

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