

## **First Principles Studies of Extrinsic and Intrinsic Defects in Boron Nitride Nanotubes**

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### **ABSTRACT**

Spin polarized density functional theory has been used to investigate the structural stability and electronic properties of extrinsic and intrinsic defects in boron nitride nanotubes. Carbon substitutional defects under nitrogen rich and boron-rich growth conditions have the lowest heats of formation compared to boron and nitrogen antisites. Creating a defect reduces the band gap of the nanotube in both armchair and zig-zag geometries. We show that the substitutional carbon atom affects the electronic properties of the nanotube in such a way that it transforms from insulator to a semiconductor or metal. Antisites are stable in the reverse atmosphere and have the main characteristic that among all defects they have the highest heats of formations in both the zig-zag and armchair nanotubes.