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First-principles studies of extrinsic and intrinsic defects in boron nitride nanotubes

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Abstract content
   (Max 300 words)

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, CB under N-rich growth condition, and CN under B-rich growth condition, presented the lowest heats of formations compared to boron and nitrogen antisites. Creating a CB defect reduces the band gap of the nanotube in both armchair and zig-zag geometries. Therefore, the substitutional carbon atom affects the electronic properties of the nanotube in such a way that it goes from insulator to a semiconductor or metal. BN in the N-rich environment and NB in the B-rich environment, have lower heats of formations, also BN and NB are stable in the reverse atmosphere and have the main characteristic is that among all defects, they present the highest heats of formations in the reverse atmospheres in both zig-zag and armchair nanotubes.

Apply to be
 consider for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

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Would you like to
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no

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