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Defect Complexes in Carbon and Boron Nitride Nanotubes

M. G. Mashapa [1, 2,*], N. Chetty [1], and S. Sinha Ray [2, 3]

[1]Physics Department, University of Pretoria, Pretoria, 0001, South Africa, and National Institute for Theoretical Physics, Johannesburg 2000, South Africa
[2]DST/CSIR Nanotechnology Innovation Centre, National Centre for Nano-Structured Materials, Council for Scientific and Industrial Research, Pretoria, 0001, South Africa
[3]Department of Chemical Technology, University of Johannesburg, Doornfontein 2018, Johannesburg, South Africa

ABSTRACT:

The effect of defect complexes on the stability, structural and electronic properties of single-walled carbon nanotubes and boron nitride nanotubes is investigated using the ab initio pseudopotential density functional method implemented in the Castep code. We found more substantial atomic relaxations in the zig-zag carbon nanotube than the armchair one. We find that the B_CB_C defect introduced in both zig-zag and armchair carbon nanotubes results in a semimetallic system. Similarly to the carbon nanotubes, the relaxation energies in the zig-zag boron nitride nanotubes are lower than in the armchair system. We find that creating a C_BB_N in the boron nitride nanotube, changes the system to metallic. The zig-zag configuration is energetically more stable than the armchair one in both the boron-rich and nitrogen-rich environments. The interaction between the carbon impurity and the antisite was investigated: we find that C_BB_N is preferable in the B-rich environment, and C_NN_B is preferable in the N-rich environment. We determine that in both zig-zag and armchair systems, B_NN_B is stable with the heats of formation of −5.77 eV and −8.69 eV, respectively.