Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Doping and Electronic Properties of Boron-Nitride Nanotubes[1]

SUSUMU SAITO, YOSHITAKA FUJIMOTO, Tokyo Instiute of Technology — We study the electronic structure of boron-nitride (BN) nanotubes in the framework of the density-functional theory. The generalized Bloch theorem for one-dimensional helical-symmetry systems is used for chiral nanotubes. It is shown that, in the case of thin nanotubes, the width of the fundamental gap depends on not only the diameter but also the chiral angle of nanotubes. We next study the electronic properties of substitutionally C-doped BN Nanotubes. In the case of the C-doped flat BN sheet, the impurity-induced states have been found to be rather deep [1]. Interestingly, in the case of BN nantoubes the ionization energy of the donor state is found to depend on the diameter, showing that the importance of the curvature for the electronic transport properties of sp^2 BN nanostructured materials. We also discuss the multiply C doped BN nanotubes with C at both B and N sites. The system shows a rich variety of electronic properties depending not only the geometry of BN nanotubes but also the relative positions of the doped sites. [1] Y. Fujimoto and S. Saito, Phys. Rev. B 93 (2016) 045402.

[1]Supported by MEXT Elements Strategy Initiative to Form Core Research Center through Tokodai Institute for Element Strategy, JSPS KAKENHI Grant Numbers JP26390062 and JP25107005.

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Date submitted: 11 Nov 2016 Electronic form version 1.4