Effects of Tube Diameter and Boron Doping on Electronic Band Structure of single-walled carbon nanotubes.

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Electronic structures of zigzag (n,0) and armchair (m,m) single-walled carbon nanotubes(SWCNT), where n being 5-23 and m being 4-8 were investigated using density functional theoretical calculations. The generalized gradient approximation (GGA) based on Perdew, Burke and Ernzerhof (PBE) functional and double numerical plus d functions (DND) basis set were employed. Calculations revealed that zigzag SWCNTs are semiconductor when n=3i and they are metal otherwise, in agreement with Saito et al.[1]. Band structures of SWCNTs were also found to be depended on type (zigzag or armchair), tube diameter (chiral vector) and Boron doping. For zigzag structures band gaps of SWCNT were observed to be increasing when n is less than 10, but the gaps decreases when n is larger than 10, similar to armchair structures for all n. With Boron doping which initiates electron deficiency center on the system, most zigzag and armchair SWCNTs turn metallic.

[1] R Saito, M. Fujita, G. Dresselhaus and M.S. Dresselhaus, Phys. Rev. B 46 (1991) 1804.