THE PROPERTIES OF BORON-CARBIDE TUBULAR STRUCTURES

O.Ponomarenko[1], M.W.Radny[1], P.V.Smith[1] and <u>G.Seifert[2]</u>

[1]*School of Mathematical & Physical Sciences, The University of Newcastle, Australia 2308*
[2]*Institut fur Physikalische Chemie, Technische Universitaet Dresden, D-01062 Dresden, Germany*

Exploration of the properties of different possible topologies for novel superconducting materials is currently one of the most promising areas in nanotechnology research. Of particular interest are recent attempts to model the properties of nanotubular analogues of layered and crystalline structures such as AlB_2 [1], $Ca(Al_xSi_{1-x})_2$ and $Sr(Ga_x Si_{1-x})_2$ [2].

LiBC is isovalent with, and structurally similar to, MgB_2 which is a novel layered superconducting compound. Rosner et al. [3] have proposed that hole doping of LiBC could shift the Fermi energy into the valence band and, in so doing, create a superconducting state. LiBC consists of hexagonal BC layers with alternating boron and carbon atoms, and a B-C bond distance of 1.55 Å. The BC layers are separated by planes of Li atoms with a Li-BC distance of 3.53 Å. Since Li is a very electropositive element, it donates its electron to the more electronegative elements B and C. The LiBC system has been modelled in the present study by taking the BC layers to be charged ($BC^{(-)}$), and treating the counter-ions ($Li^{(+)}$) as a homogeneously distributed background charge. This modelling produces $BC^{(-)}$ structures which are isoelectronic to LiBC. We have also considered hole-like doping of $BC^{(-)}$ by reducing the charge per boron-carbon pair from –e to –0.5e [3].

In this paper we report the results of calculations performed on these BC tubes using the Density Functional Tight-Binding (DFTB) method [4]. These calculations have shown that negatively charged Boron-Carbide ($BC^{(-)}$) nanotubes are stable and energetically viable. Moreover, these $BC^{(-)}$ tubes are semiconducting, with the size of the energy gap being dependent on both the helicity and diameter of the tubes. We have also found, in agreement with results of Rosner et. al [3] for layered LiBC, that hole doping of $BC^{(-)}$ nanotubes makes these systems metallic.

[1] A. Quandt, A.Y. Liu and I. Boustani, Phys. Rev. B **64** 2001) 125422.
[2] I.R. Shein, V.V Ivanovskaya, N.I. Medvedeva and A.L. Ivanovskii, JETP Lett. **76** (2002) 189.
[3] H. Rosner, A. Kitaigorodsky and W. E. Pickett, Phys. Rev. Lett. **88** (2002) 127001.
[4] D. Porezag *et. al.*, Phys. Rev. B **51** (1995) 12947.