Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First Principles Study of Nanotubes of Boron. KAH CHUN LAU, RANJIT PATI, RAVINDRA PANDEY, Michigan Technological University, Houghton, MI — Current trends in miniaturization of electronic devices have motivated a growing interest in various nanoscale structures. Besides carbon nanotubes, boron nanotubes are believed to be another stable "homonuclear" nanotubes, which has recently been synthesized. Understanding of the structural stability, electronic properties and chemical bonding of boron nanotubes can be set as another baseline for the evolutionary changes from carbon nanotubes to hybrid $C_xB_yN_z$ nanotubes to boron-nitride nanotubes. We will present the results on structural stability, electronic properties and chemical bonding of boron nanotubes using first principles periodic approach. Specifically, we will discuss the configurational stability and dependence of the band structure on the diameter of the boron nanotubes.

Ravindra Pandey
Michigan Technological University, Houghton, MI

Date submitted: 23 Nov 2004 Electronic form version 1.4