Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Negative curvature energy in magnesium-boride nanotubes HUI TANG, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Mg-boride nano-materials have attracted much attention due to constant quest for novel superconducting materials on nanoscale. A recent experiment on Mg borides nanostructures has hinted at a possible superconducting temperature as high as 80K. More generally, studying the physics of pure and metal-doped boron nanosystems enhances understanding of novel properties that emerge in reduced dimensions. Here, based on first principles calculations, we describe an unusual nanoscale curvature effect in Mg-boride nanotubes and discuss its origin. We show that a number of 2D Mg-boride sheets prefer to spontaneously curve themselves into small diameter nanotubes and thus have negative curvature energies. This is rather unique when compared to other nanotubular materials: usually, curving the parent 2D sheet to create a nanotube imposes an energy cost. We explain the reason for the negative curvature energy by analyzing the charge state of the Mg atoms, its relation to the type of boron sublattice present in the nanostructure, and its consequences for the Mg-Mg interactions and hence the energetics.

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Date submitted: 18 Nov 2010 Electronic form version 1.4