

Abstract Submitted
for the TSF09 Meeting of
The American Physical Society

Borozone: A Building Block of Boron Nanostructures NEVILL GONZALEZ SZWACKI, Texas Southern University, VALERY WEBER, University of Zurich, CHRISTOPHER J. TYMCZAK, Texas Southern University — Bulk boron exhibits a complex crystal structure due to its electron-deficient bonds, and in all known forms is semiconducting. However, there is little known about the properties of boron at the nanometer scale. For example, it has been experimentally reported that boron can form nanotubes that are metallic; however, the structure of these nanotubes remains still unknown [1]. Based on first principles calculations we present a theoretical investigation on the structure and electronic properties of all-boron and boron related nanostructures. Special emphasis will be placed on our recent work [2] on the theoretical identification of an unusually stable planar molecule, B₁₂H₆, which has similar structural and electronic properties to the well-known benzene. We investigate this molecule as a promising building block of boron hollow nanoclusters and nanotubes.

[1] D. Ciuparu, R. F. Klie, Y. Zhu, L. D. Pfefferle, *Journal of Physical Chemistry B* 108, 3967 (2004)

[2] N. Gonzalez Szwacki, V. Weber, and C. J. Tymczak, *Nanoscale Res. Lett.* 4, 1085 (2009).

Nevill Gonzalez Szwacki
Texas Southern University

Date submitted: 02 Oct 2009

Electronic form version 1.4