Abstract Submitted
for the APR12 Meeting of
The American Physical Society

Dispersion corrections in the boron buckyball and nanotubes[1]
ROSI GUNASINGHE, CHERNO KAH, KREGG QUARLES, XIAO-QIAN WANG, Clark Atlanta University — We have investigated structural and electronic properties of the B_{80} buckyball and boron nan-otubes by means of dispersion-corrected density-functional calculations. Our analysis reveals the vibrational stability for the icosahedral B_{80} with the inclusion of dispersion corrections, in contrast to the instability to a tetrahedral B_{80} with puckered capping atoms from preceding density-functional theory calculations. Similarly, the dispersion-corrected density-functional calculations yield non-puckered boron nanotube conformations and an associated metallic state for zigzag tubes. Our study indicates that the incorporation of long-range dispersive interactions is particularly important to the structural and electronic properties of boron fullerenes and nanotubes.

[1]This work was supported by the National Science Foundation (Grant No. DMR-0934142), Army Research Office (Grant No. W911NF-10-1-0302), and Air Force office of Scientific Research (Grant No. FA9550-10-1- 0254).

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Date submitted: 11 Jan 2012 Electronic form version 1.4