Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Structural, Elastic, and Electronic Properties of Deformed Carbon Nanotubes under Uniaxial Strain A. PULLEN, Southern University and A & M College and California Institute of Technology , G.L. ZHAO, D. BAGAYOKO, Department of Physics, Southern University and A & M College, Baton Rouge, LA 70813, L. YANG, NASA Ames Research Center — We report structural, elastic, and electronic properties of selected, deformed, single-wall carbon nanotubes under uniaxial strain. We utilized a generalized gradient approximation (GGA) potential of density functional theory and the LCAO formalism. We discuss bond-lengths, tubule radii, and the band gaps as functions of tension and compression strain for carbon nanotubes (10, 0), (8, 4) and (10, 10) which have chiral angles of 0, 19.1, and 30 degrees relative to the zigzag direction. We also calculated the Young's modulus and the in-plane stiffness for each of these three nanotubes as representatives of zigzag, chiral, and armchair nanotubes, respectively. We found that these carbon nanotubes have unique structural properties consisting of a strong tendency to retain their tubule radii under large tension and compression strains. Work funded in part by US NASA (Award No. NCC 2-1344).

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Date submitted: 02 Dec 2004 Electronic form version 1.4