Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Electronic structure of Defective and Deformed Single Wall Carbon Nanotubes L.M. WOODS, YA. SHTOGUN, Department of Physics, University of South Florida, T.L. REINECKE, Naval Research Laboratory, Washinton DC — Carbon nanotube properties can be modified by the introduction of defects on their surface or by mechanical deformations. Here we present an alternative way to modify carbon nanotube characteristics by considering both types of mechanical alterations, defects and deformations, on the nanotube surface. Electronic structure calculations from first principle density functuional theory using the VASP code (Viena Ab initio Simulations Package) for metallic and semiconducting single walled carbon nanotubes with Stone-Wales defect and radial deformation are presented. The difrferent degrees of deformation and various defect locations are analyzed in terms of the density of states and bandstructures of these systems. We compare the defective and deformed nanotube electronic structure to the electronic structure of only defective or only deformed nanotubes. In this way we determine the relative importance of the two types of mechanical alterations on the defective and deformed nanotubes.

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Date submitted: 20 Nov 2006 Electronic form version 1.4