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Pressure Induced Changes in the Atomic and Electronic Structure of Carbon Nanotubes SUMIT SAXENA, TREVOR A. TYSON, New Jersey Institute of Technology - Newark — We present first principle density functional calculations on small diameter single walled carbon nanotubes to explore the changes in their electronic structure and atomic arrangement under hydrostatic compression. Simulations on zigzag (n, 0) SWCNT $6 \leq n \leq 9$ using the full potential projector augmented wave and ultra-soft pseudo potentials were conducted. Large structure-related changes are found in the density of states at the Fermi energy. The cross sections of small tubes exhibits deformations not predicted by classical models. The structural cross sections of large diameter tubes[1] (10, 0) calculated under moderate pressure are consistent with the reported results. The details of calculations and other results will be presented. This work is supported in part by NSF DMR-0512196.

1. Paul Tangney, Rodrigo B. Capaz, Catalin D. Spataru, Marvin L. Cohen and Steven G. Louie, Nano Lett. 5, 2268 (2005).

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