Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Quantum Manifestations of Graphene Edge Stress and Edge Instability[1] BING HUANG, Department of Physics, Tsinghua UniVersity, MIAO LIU, NINGHAI SU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, Utah 84112, USA, JIAN WU, WENHUI DUAN, Department of Physics, Tsinghua UniVersity, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, Utah 84112, USA — We have performed first-principles calculations of graphene edge stresses, which display two interesting quantum manifestations absent from the classical interpretation: the armchair edge stress oscillates with nanoribbon width and the zigzag edge stress is noticeably reduced by spin polarization [1]. Such quantum stress effects in turn manifest in mechanical edge twisting and warping instability, showing features not to be captured by empirical potentials or continuum theory. Edge adsorption of H and Stone-Wales reconstruction are shown to provide alternative mechanisms in relieving the edge compression and hence to stabilize the planar edge structure. We also demonstrate that the quantum manifestation of mechanical properties such as stress to exist generally in many low-dimensional nanostructures, such as BN system.
[1] Huang et al., Phys. Rev. Lett. 102, 166404 (2009).

[1]The work at Beijing is supported by NSFC, and the work at Utah was supported by DOE

Bing Huang
Department of Physics, Tsinghua UniVersity

Date submitted: 01 Dec 2009 Electronic form version 1.4