Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Analysis of band-gap formation in squashed armchair CNTs H. MEHREZ, A. SVIZHENKO, M. P. ANANTRAM, Mail Stop: 229-1, Center for NanoTechnology and NASA Advanced Supercomputing Division, NASA Ames Research Center, Moffett Field, California 94035-1000, M. ELSTNER, T. FRAUENHEIM, heoretische Physik, Universitat Paderborn, D-33098 Paderborn, Germany —
The electronic properties of squashed arm-chair CNTs are modeled using constraint free density functional tight binding molecular dynamics simulations. Independent from CNT diameter, squashing path can be divided into *three* regimes. In the first regime, the CNT deforms with negligible force. In the second one, there is significantly more resistance to squashing with the force being $\sim 40 - 100$ nN/per CNT unit cell. In the last regime, the CNT looses its hexagonal structure resulting in force drop-off followed by substantial force enhancement upon squashing. We compute the change in band-gap (E_g) as a function of squashing and our main results are: (i) E_g initially opens due to interaction between atoms at the top and bottom sides of CNT. The $\pi-$orbital approximation is successful in modeling the E_g opening at this stage. (ii) In the second regime of squashing, large $\pi - \sigma$ interaction at the edges becomes important, which can lead to E_g oscillation. (iii) Contrary to a common perception, nanotubes with broken mirror symmetry can have *zero* E_g. (iv) All armchair nanotubes become metallic in the third regime of squashing.[Phys. Rev. B 71, 155421 (2005)]

H. Mehrez
NanoTechnology Ctr., NASA Ames Res. Ctr.

Date submitted: 06 Jan 2006 Electronic form version 1.4