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Analysis of band-gap formation in squashed arm-chair CNT H. MEHREZ, A. SVIZHENKO, M.P. ANANTRAM, NASA AMES Res. Ctr., Moffett Field, CA 94035, M. ELSTNER, T. FRAUENHEIM, Theoretische Physik, Universitat Paderborn, D-33098 Paderborn, Germany — The electronic properties of squashed arm-chair carbon nanotubes are modeled using constraint free density functional tight binding molecular dynamics simulations. Independent from CNT diameter, squashing path can be divided into three phases. In the first phase of squashing, the nanotube deforms with negligible force. In the second phase, there is significantly more resistance to squashing with the force being 40-100nN/per CNT unit cell, and in the last phase the nanotube loses its hexagonal configuration. We compute the change in band-gap as a function of squashing and our main results are: (i) A band-gap initially opens due to interaction between atoms at the top and bottom sides of CNT. The Pi-orbital approximation is successful in modeling the band-gap opening at this stage. (ii) In the second phase of squashing, large Pi-Pi* interaction at the edges becomes important, which can lead to band-gap oscillation. (iii) Contrary to a common perception, nanotubes with broken mirror symmetry can have zero band-gap. (iv) All arm-chair nanotubes become metallic in the third phase of squashing. Finally, we discuss both differences and similarities obtained from the tight binding and density functional approaches.

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