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The Influence of Uniaxial, Radial and Torsional Deformations on the Electronic Properties of Nanotubes: An O(N) TBMD Study

Cem Ozdogan[b], Gulay Dereli[b], Tahir Cagin[*, a]

[a]*Materials and Process Simulation Center, MS 139-74, California Institute of Technology, Pasadena, CA 91125, USA*

[b]*Department of Physics, Middle East Technical University 06531 Ankara, TURKEY*

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Due to their novel mechanical and electronic properties, carbon nanotubes are perceived to play a major role in the design of next generation nanoelectronic, nanoelectromechanical devices. The conductivity behaviour of single wall nanotubes is mostly determined by the chirality of the tubes. Depending on their chirality, they could be conductor, semiconductor as well as insulators. It is now widely known that the conductivity of the tubes may also change due to presence of defects (pentagonal, heptagonal topological defects, substitutional impurities) as well as radial deformations. Deformations such as uniaxial compressive/tensile or torsional will also modify the band gap of the nanotubes and under such deformations single wall carbon nanotubes undergo conducting-semiconducting-insulator transitions. Using O(N) parallel tight binding molecular dynamics method we study the electronic structure of nanotubes with diameters upto 2 nm. In this talk we will report on the band structure, transitions, density of states of SWNT at elevated temperatures.

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*Corresponding Address:
Tahir Cagin
Materials and Process Simulation Center, MS 139-74
California Institute of Technology
1200 E. California Blvd
Pasadena, CA 91125, USA
Email: tahir@wag.caltech.edu
Web: http://www.wag.caltech.edu/home/tahir/